*ANS RPSD 2018 - 20th Topical Meeting of the Radiation Protection & Shielding Division of ANS*
Santa Fe, NM, August 26 – 31, 2018, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2018)

# APPLICATION OF POLYNOMIAL CHAOS EXPANSION IN INVERSE TRANSPORT PROBLEMS WITH NEUTRON MULTIPLICATION MEASUREMENTS AND MULTIPLE UNKNOWNS

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*The polynomial chaos expansion technique is used to build surrogate models of the dependences of gamma-ray fluxes and neutron multiplication to unknown physical parameters in radiological source/shield systems. These surrogate models are used with the DiffeRential Evolution Adaptive Metropolis (DREAM), a method to solve and quantify uncertainty in inverse transport problems. Measured data in the inverse problems includes both passive gamma rays and neutron multiplication. The polynomial chaos expansion approach is shown to increase the speed of DREAM by factors of greater than 60 while not degrading the accuracy of the solution.*

## I. INTRODUCTION

In the problem of inverse radiation transport, measurements of particle leakages from radioactive source/shield systems are used to infer unknown parameters within the systems. This reconstruction can be accomplished by finding the physical parameters of the unknown system that minimize the difference between calculated detector responses and measured detector responses. The inverse transport solver should also propagate uncertainties from the detector responses to the reconstructed parameter values. Recently, the DiffeRential Evolution Adaptive Metropolis (DREAM) method, an advanced Markov chain Monte Carlo (MCMC) approach, was shown to be a robust method for uncertainty quantification in inverse problems.[1] Although DREAM is more efficient than traditional MCMC approaches, it still requires thousands of transport computations to accurately quantify uncertainty. Therefore, inverse transport problems that require computationally intensive transport solvers will need prohibitively long run times when using the DREAM method. It has previously been demonstrated that the polynomial chaos expansion method reduces by orders-of-magnitude the number of transport calculations required by the DREAM method for solving inverse transport problems with passive gamma-ray measurements and a single unknown parameter.[2] This work constitutes an expansion of such analysis to problems with multiple unknown parameters and to those that use neutron multiplication as well as passive gamma-ray measurements.

## II. DREAM METHOD AND POLYNOMIAL CHAOS EXPANSION (PCE)

### II.A. DREAM Method

MCMC simulations provide a generalized methodology for obtaining the posterior distribution of the unknown parameters in an inverse transport problem. For a vector $\mathbf{u}$ representing postulated values for unknown parameters, this posterior distribution, $p(\mathbf{u}|M_o)$, represents the probability of a model $\mathbf{u}$ (), given observed measurements $M_o$ . Following Bayes Theorem, this distribution is proportional to the product of likelihood function and a prior probability distribution. For this study, a uniform prior distribution between the physical constraints of the parameter was assumed. This indicates that there is no *a priori* information about the parameter's value. Other distributions could be used when prior knowledge is available. As with previous work,[2] the likelihood function was defined as

$$p(M_o|\mathbf{u}) = \exp\left[-\frac{1}{2}\sum_{d=1}^{D}\left(\frac{M_d(\mathbf{u}) - M_{d,o}}{\sigma_d}\right)^2\right], \quad (1)$$

where $D$ is the total number of detector measurements, $M_d(\mathbf{u})$ is the calculated response for detector $d$ for the postulated parameter set $\mathbf{u}$ , $M_{d,o}$ is the observed measurement for detector $d$, and $\sigma_d$ is the uncertainty in the measurement for detector $d$. The goal of the inverse problem is to find the regions for which $p(M_o|\mathbf{u})$ is at or near its maximum.

In the traditional MCMC approach, a single Markov chain is employed. The chain begins at some initial parameter values $\mathbf{u}_t$ ,for which $p(\mathbf{u}_t|M_o)$ is calculated. After this, trial values for the unknown parameters are created using an updating technique, several of which have been presented in the last few decades.[3] These techniques range from simple methods like sampling from Gaussian distributions centered about the initial trial values to the use of evolutionary algorithms. The posterior distribution $p(\mathbf{u}_{t+1}|M_o)$ is calculated for the trial parameter values, and the trial set is either accepted or rejected according to the Metropolis acceptance probability:[4]

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$$\alpha(\mathbf{u}_t, \mathbf{u}_{t+1}) = \min\left[\frac{p(\mathbf{u}_t|M_o)}{p(\mathbf{u}_{t+1}|M_o)}, 1\right]. \quad (2)$$

According to Eq. (2), if the trial point has a posterior smaller than the current chain state (i.e., parameters $\mathbf{u}_{t+1}$ yield a closer match between calculated and observed measurements), then the acceptance probability is 1, and the chain is moved to the trial state. If parameters $\mathbf{u}_{t+1}$ do not lead to a closer match between calculated and observed measurements, they could still be accepted, with a probability equal to $p(\mathbf{u}_t|M_o)/p(\mathbf{u}_{t+1}|M_o)$. The chain progresses in this way until it creates the full posterior distribution describing the probabilities for the values of the unknown parameters.

Traditional MCMC approaches have generally been inefficient because many of the traditional updating schemes create trial parameters are either too close to the current point, leading to a high acceptance rate but slow convergence to the posterior distribution, or they are too far from the current point, leading to a low acceptance rate. The issue of choosing trial parameters has been explored for many years. The DREAM algorithm has been particularly successful at finding appropriate trial parameters. DREAM has been shown to greatly increase the speed of the MCMC process and to be highly successful for solving difficult optimization problems in the presence of noise.[4] DREAM also employs simultaneous multiple Markov chains (generally 3–5) and uses the differential evolution (Ref. 5) algorithm to generate trial points for each chain. In the case of multiple chains, the Metropolis ratio [Eq. (2)] becomes

$$\alpha\left(\mathbf{u}_1, \ldots, \mathbf{u}_N; \mathbf{u}_{1,trial}, \ldots, \mathbf{u}_{N,trial}\right) = \min\left[\frac{p(\mathbf{u}_1|M_o) + \cdots + p(\mathbf{u}_N|M_o)}{p\left(\mathbf{u}_{1,trial}|M_o\right) + \cdots + p\left(\mathbf{u}_{N,trial}|M_o\right)}, 1\right]. \quad (3)$$

When applying MCMC algorithms, a stopping point must be determined. This work implements the Gelman–Rubin convergence metric (Ref. 6) to automatically detect when the posterior distribution has been sufficiently sampled. This diagnostic compares the estimated between-chains and within-chain variances. When these variances are similar, then the multiple chains have all converged to the same region and are (ideally) sampling the posterior distributions of the unknown parameters.

### II.B. Polynomial Chaos Expansion (PCE)

Each computation of the likelihood function [Eq. (1)] requires calculation of $M_d(\mathbf{u})$ the quantities of interest (QOI) (gamma-ray flux or neutron multiplication) that corresponds to a set of postulated values for the unknown parameters. PCE is used to create a surrogate model for these QOIs. First consider the case where the QOI is a function of one unknown parameter (an internal dimension, source enrichment, etc.) that can be described by a uniformly distributed random variable $\xi_1$ over some interval. This could, for example, be a source radius whose exact location is unknown but is known to be between 0 cm and 10 cm. The QOI as a function of the unknown parameter, $\psi(\xi_1)$, can be expressed as a continuous polynomial over this interval. To do this, Legendre polynomials $\{P_0(\xi_1), P_1(\xi_1), \ldots\}$are employed, which form a set of basis functions for continuous polynomials on $[-1,1]$ and can (with linear translation) be used over other closed intervals. The orthogonal projection can be shown to be the best approximation of $\psi$ in the Legendre polynomial basis.[7] The projection of $\psi(\xi_1)$ onto the Legendre polynomial basis is given by

$$\psi(\xi_1) \approx \sum_{i=0}^{K} a_i P_i(\xi_1), \quad (4)$$

where the deterministic coefficients $a_i$ are obtained by applying the orthogonality of the Legendre polynomials

$$a_i = \frac{\langle \psi(\xi_1), P_i(\xi_1)\rangle}{\langle P_i(\xi_1), P_i(\xi_1)\rangle}. \quad (5)$$

Equation (4) is called the polynomial chaos expansion of $\psi$.

The denominator of Eq. (5) is determined by the orthogonality property of the Legendre polynomials, which is

$$\int_{-1}^{1} d\xi_1 P_i(\xi_1) P_j(\xi_1) = \frac{2}{2i+1}\delta_{ij}\,. \quad (6)$$

The numerator can be solved by performing a numerical integration with Gauss–Legendre quadrature:

$$\langle \psi(\xi_1) P_i(\xi_1)\rangle \approx \sum_{n=1}^{N} w_n \psi(\xi_{1,n}) P_i(\xi_{1,n}), \quad (7)$$

where the $w_n$ are weights of the quadrature points, $\xi_{1,n}$ is the $n^{\text{th}}$ abscissa of the quadrature set, and $\psi(\xi_{1,n})$ is the measured quantity at parameter value $\xi_{1,n}$, which is determined by a transport calculation. Using this approach, an approximation for the QOI in terms of the PCE of $\xi_1$ in Eq. 4 can be constructed with $N$ transport computations.

Now consider a QOI $\psi(\xi_1, \xi_2)$ as a function of two unknown parameters, each of which can be represented by uniformly distributed variables. In two dimensions the basis is the tensor product of the individual bases for the random variables. Again using Legendre polynomials for each variable, the individual bases are $\{P_0(\xi_1), P_1(\xi_1), \ldots\}$

and $\{P_0(\xi_2), P_1(\xi_2) \ldots\}$. To obtain the basis functions for a 2nd-order expansion in two dimensions, the tensor product of the two bases is computed and terms that have a total order of 2 or less are selected: $P_0(\xi_1)P_0(\xi_2)$, $P_0(\xi_1)P_1(\xi_2)$, $P_0(\xi_1)P_2(\xi_2)$, etc. Using these terms, the 2nd-order expansion is:

$$\begin{aligned}\psi(\xi_1,\xi_2) \approx a_{00}P_0(\xi_1)P_0(\xi_2) &+ a_{10}P_1(\xi_1)P_0(\xi_2)\\ &+ a_{01}P_0(\xi_1)P_1(\xi_2)\\ &+ a_{11}P_1(\xi_1)P_1(\xi_2)\\ &+ a_{20}P_2(\xi_1)P_0(\xi_2)\\ &+ a_{02}P_0(\xi_1)P_2(\xi_2).\end{aligned} \quad (8)$$

The procedure can be generalized to generate 3rd-order or higher-order expansions.

The coefficients $a_{ij}$ in Eq. (8) are again determined using the orthogonality property of the Legendre polynomials, for instance

$$a_{00} = \frac{\langle \psi(\xi_1,\xi_2)P_0(\xi_1)P_0(\xi_2)\rangle}{\langle P_0^2(\xi_1)P_0^2(\xi_2)\rangle} = \frac{\langle \psi(\xi_1,\xi_2)\rangle}{\langle 1\rangle} \quad (9)$$

and

$$a_{10} = \frac{\langle \psi(\xi_1,\xi_2)P_1(\xi_1)P_0(\xi_2)\rangle}{\langle P_1^2(\xi_1)P_0^2(\xi_2)\rangle} = \frac{\langle \xi_1\psi(\xi_1,\xi_2)\rangle}{\langle \xi_1^2\rangle}. \quad (10)$$

The denominators of the equations for $a_{ij}$ admit analytical solutions by performing integrals of the form

$$\int_{-1}^{1} d\xi_1 \int_{-1}^{1} d\xi_2\, P_i^2(\xi_1)P_j^2(\xi_2). \quad (11)$$

The numerators can be solved numerically using Gauss–Legendre quadrature:

$$\begin{aligned}&\langle \psi(\xi_1,\xi_2)P_i(\xi_1)P_j(\xi_2)\rangle\\ &\approx \sum_{m=1}^{M}\sum_{n=1}^{N} w_m w_n \psi(\xi_{1,m},\xi_{2,n})P_i(\xi_{1,m})P_j(\xi_{2,n}).\end{aligned} \quad (12)$$

In Eq. (12), $w_m$ and $w_n$ are weights of the quadrature points, $\xi_{1,m}$ is the $m^{\text{th}}$ abscissa of the quadrature set for the first variable, $\xi_{2,n}$ is the $n^{\text{th}}$ abscissa of the quadrature set of the second variable, and $\psi(\xi_{1,m},\xi_{2,n})$ is the QOI at unknown parameter values $\xi_{1,m}, \xi_{2,n}$, which is determined by a transport calculation. An approximation for the QOI can therefore be constructed using $M \times N$ transport computations. Coefficients for higher-order expansions are calculated in a similar manner.

PCE is implemented into the DREAM method by using the surrogate model in place of $M_d(\mathbf{u})$ in Eq. (1). Consequently, the DREAM method with PCE requires only the number of transport calculations necessary to build the surrogate model.

## III. NUMERICAL RESULTS

### III.A Background

To demonstrate the method, both one-dimensional (spherical) and two-dimensional (cylindrical) test cases were considered. The test cases contain a uranium source for which neutron multiplication can be measured. The source also emits several discrete gamma-ray lines, including one at 1,001 keV. In the test problems, a PCE surrogate model was constructed for neutron multiplication and for the leakage (spherical problem) or flux (cylindrical problem) of the 1,001-keV gamma-ray line at the detector point (so that there would be two unknowns and two QOIs). Measured values were simulated using the same ray-tracing routine used by the DREAM algorithm, meaning there was no measurement uncertainty (the focus of this work is on improving computational speed rather than quantifying all sources of uncertainty).

### III.B. Spherical Geometry

The first test case was performed using the spherical geometry shown in Fig. 1. A highly enriched uranium source with a radius of 8.741 cm was surrounded by layers of lead and aluminum shielding. The shielding had an inner radius of 12.40 cm. The unknown parameters were the source radius and the inner shield radius.

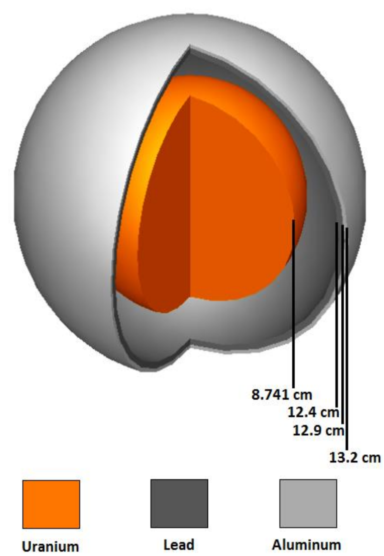


Fig. 1. Geometry for the spherical test problem

The first test case results are provided in Table I. Fifth-order PCE expansions were used to build surrogates for the flux and multiplication, requiring a total of 36 transport calculations (here "transport calculation" refers to both the calculation of the gamma-ray flux and the neutron multiplication). The fifth-order expansion was determined by trial-and-error. Expansions of increasingly higher order were tried until the DREAM with PCE results matched standard DREAM results to better than 99.9%. The time required to build these surrogates was 190 seconds (DREAM itself required less than 1 second of computation time when using the surrogates). DREAM with PCE obtained virtually identical results to standard DREAM, which required 9,790 transport calculations and 15,000 seconds of run time. Thus, DREAM with PCE was a factor of 79 faster than standard DREAM.

### III.C. Cylindrical Geometry

The second numerical test problem was performed with the geometry shown in Fig. 2. A cylindrical source of highly enriched uranium has a radius of 4.0 cm and a height of 4.5 cm; it was surrounded by layers of nickel and aluminum shielding. Detectors at $(r, z) =$ (10.0 cm, 4.0 cm) measured the flux of the 1,001-keV gamma-ray line and the neutron multiplication. The unknown parameters in this problem were the source radius and axial location of the top of the source (actual value 6.0 cm).

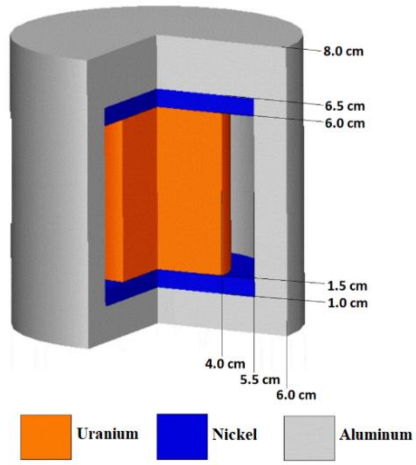


Fig. 2. Geometry for the cylindrical test problem

The second test case results are provided in Table II. A 9th-order PCE expansion, requiring 100 transport calculations, was required to produce results with the required accuracy of 99.9%. DREAM with PCE required 84 minutes to solve the problem and obtained a solution very similar to standard DREAM, which required 6,132 transport calculations and 5,160 minutes of run time. DREAM with PCE was thus a factor of 54 faster than standard DREAM.

TABLE I: DREAM Results for the Spherical Test Problem

| Parameters | Method | DREAM Result | Transport Calculations | Run Time (s) | Speedup Factor |
|---|---|---|---|---|---|
| Source Radius<br>Inner Shield Radius | Standard DREAM | 8.741 ± 0.001 cm<br>12.40 ± 0.001 cm | 9,790 | 15,000 | — |
| Source Radius<br>Inner Shield Radius | DREAM with PCE | 8.742 ± 0.003 cm<br>12.40 ± 0.002 cm | 36 | 190 | 79 |

TABLE II: DREAM Results for the Cylindrical Test Problem

| Parameters | Method | DREAM Result | Transport Calculations | Run Time (min) | Speedup Factor |
|---|---|---|---|---|---|
| Source Radius<br>Source Top | Standard DREAM | 4.02 ± 0.11 cm<br>5.99 ± 0.27 cm | 6,132 | 5,160 | — |
| Source Radius<br>Source Top | DREAM with PCE | 3.99 ± 0.10 cm<br>6.01 ± 0.29 cm | 100 | 84 | 61 |

## IV. CONCLUSIONS

The PCE method has been used to build surrogate models of measured quantities in inverse transport problems with measurements of passive gamma rays and neutron multiplication. These surrogates were used in the DREAM method to find the unknown parameters. In numerical test cases, DREAM with PCE was shown to be over a factor of 61 faster than standard DREAM for problems with two unknown parameters.

Several areas of future research remain for DREAM with PCE. In the numerical test problems, PCE expansion orders of 5 and 9 were manually determined to be the minimum expansion orders necessary to obtain accurate solutions. A current area of study is to automatically determine the optimal PCE order. Another current research thrust is to quantify the error introduced by the surrogate models.

For problems with more (3 or more) unknown parameters, the cost of building the surrogate function can become more expensive than using the standard DREAM method. A way to reduce this cost is to use sparse grid quadrature sets rather than Gauss–Legendre quadrature sets in Eq. (12). This is also a current area of study.

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