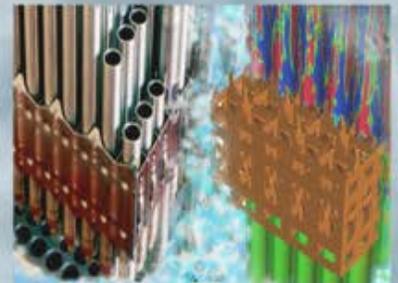
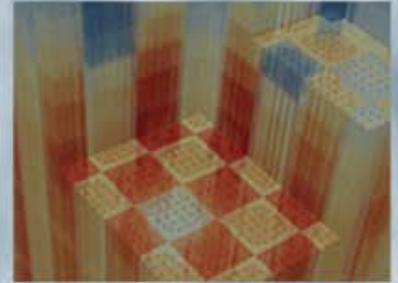


# CRANE: A New Scale Super-Sequence for Neutron Transport Calculations

Congjian Wang and Hany S. Abdel-Khalik  
Purdue University

Ugur Merturek  
Oak Ridge National Laboratory

**March 29, 2015**



## **CRANE: A NEW SCALE SUPER-SEQUENCE FOR NEUTRON TRANSPORT CALCULATIONS**

**Congjian Wang and Hany S. Abdel-Khalik**  
School of Nuclear Engineering, Purdue University  
[wang1730@purdue.edu](mailto:wang1730@purdue.edu); [abdelkhalik@purdue.edu](mailto:abdelkhalik@purdue.edu)

**Ugur Mertyurek**  
Oak Ridge National Laboratory  
[mertyureku@ornl.gov](mailto:mertyureku@ornl.gov)

**Keywords:** Reduced order modeling, intersection subspace method, EpGPT

### **ABSTRACT**

A new “super-sequence” called CRANE has been developed to automate the application of reduced order modeling (ROM) to reactor analysis calculations under the SCALE code environment. This new super-sequence is designed to support computationally intensive analyses that require repeated execution of flux solvers with variations in design parameters and nuclear data. This manuscript provides a brief overview of CRANE and demonstrates its applications to representative reactor physics calculations. Specifically, two ROM applications are demonstrated, the intersection subspace-based approach for uncertainty quantification which is intended to reduce the number of uncertainty sources in a conventional uncertainty analysis, and the exact-to-precision generalized perturbation theory methodology intended as a physics-based surrogate model to replace the flux solver, i.e., NEWT. Our overarching goal is to provide a prototypic ROM capability that allows users to further explore and investigate the benefits of using ROM methods in their respective domain and help guide further developments of the methodology and evolution of the tools.

### **1. INTRODUCTION**

This manuscript introduces a new “super-sequence” CRANE, Complexity Reduction Algorithms in Nuclear Engineering calculation, in SAMPLER under scale6.2 beta2 designed to enable the application of ROM for large-scale engineering calculations as well as to reduce the run-time of reactor physics calculations via ROM. CRANE implements some of the recent developments in the area of ROM, such as intersection subspace-based uncertainty quantification (UQ)<sup>1</sup>, and exact-to-precision generalized perturbation theory (EpGPT)<sup>2</sup>. CRANE automates all the steps related to the implementation of ROM techniques, such as subspace construction, dominant parameters identification/ranking, and surrogate model construction. The SAMPLER super-sequence is leveraged by CRANE to perform some of the tasks related to the introduction of

parameter perturbations, preparation of the associated perturbed input files, and the subsequent submission of code runs in a parallel environment<sup>3</sup>.

ROM has been developed to address a basic challenge in reactor analysis calculations - that is the need to evaluate the dependence of the flux spectrum on the many conditions of interest to the application. For example, to perform core-wide calculations, one must generate few-group cross-sections that are functionalized in terms of many core conditions that affect the neutron spectrum, e.g., fuel temperature, coolant voiding or temperature, boron poison, control rod insertion, etc. Other applications such as nuclear fuel transport and final storage also require many flux evaluations to properly characterize the fuel inventory. The flux solver in SCALE is known to be few orders of magnitude slower than comparable codes used in the industry. Hence, this manuscript will demonstrate the application of ROM techniques to generate a surrogate model that can be used in lieu of NEWT for the wide range analysis conditions. This serves as a demonstration of the capability of ROM techniques, which has general applicability to other flux solvers.

The fundamental idea behind ROM is to reduce the effective dimensionality of the associated space, e.g., parameter space, flux space, response space, etc. The reduction is rendered via a linear mapping between the original space variables and a set of reduced variables referred to the active degrees of freedom (DOFs). Due to the nature of linear mapping, the reduction identifies an active subspace that has a much fewer DOFs than the original space. The premise is that the active subspace captures the majority of the dominant effects, whereas all DOFs that are orthogonal to the active subspace are considered to have negligible impact on the responses of interest and the flux. Because the active subspace is generated using a randomized approach, the resulting reduction errors can be rigorously quantified.

ROM first appeared in 1970s dealing with linear/nonlinear structural analysis, and since then have been employed and further developed by many researchers from different scientific backgrounds, e.g., fluid dynamics, nuclear physics, and quantum mechanics<sup>4,5</sup>. The essential approach utilized to construct ROM is known as proper orthogonal decomposition (POD) or POD of snapshots. A snapshot is denoted as the outputs of a model at a particular point in time or for a given parameters perturbation. In our recent development, we have shown that the POD of snapshots (and randomized range finding algorithms (RFAs), defined later) can be employed to identify an active subspace that approximates the dominant variations of responses of interest to a quantifiable accuracy with high probability<sup>6</sup>. This is one of the main advantages of ROM techniques over conventional surrogate methods which employ parametric functional approximations to replace the original physics model, such as polynomial chaos techniques, and stochastic collocation methods. For more details on the differences between ROM and parametric functional approximation techniques, see Ref. [7]

The EpGPT approach has been developed to allow for a practical use of exact generalized perturbation theory in routine design reactor calculations. EpGPT first employs ROM to reduce the effective dimensionality of the flux space. Next, it recasts the GPT equations in terms of the identified active DOFs resulting from the reduction. Finally, it

employs a recursive approach to combine all higher order response variations to arrive at an analytical form that can be used as a surrogate model. The constructed surrogate provides an enabling tool to analyze the impact of parameters variations on the responses of interest as many times as needed without having to re-execute the original flux solver, i.e., NEWT.

With regard to the subspace-based UQ approach, this approach is designed to first identify the dominant active DOFs in the parameter space prior to the execution of conventional UQ analysis. If the active DOFs are few, one can employ forward UQ techniques to determine both uncertainties and sensitivities, i.e., contribution of the various parameters to the total propagated uncertainties. Note that in this case the active subspace represents an intersection between the active subspace for the surrogate model and the Karhonen-Loeve subspace determined from a rank revealing decomposition of the cross-section covariance matrix. This is because the propagated uncertainties are determined by the product of sensitivities of responses and uncertainties of input parameters. The key or dominant parameter directions contributing the most to the propagated uncertainties are expected to have a high net product of sensitivities and uncertainties. This criterion implies that parameter directions that are associated with strong sensitivities may not have a dominant impact on the propagated uncertainties unless their associated uncertainties are relatively high as well.

## 2. METHODOLOGY AND IMPLEMENTATION

### 2.1 EpGPT Surrogate Model Construction

The main difference between EpGPT and standard GPT theory<sup>9</sup> is in the formulation and interpretation of the adjoint models employed to calculate responses variations. GPT calculates an adjoint function for the response of interest which can be used to calculate the first order derivatives of the given response with respect to all model parameters. If higher order variations are required, one must calculate additional number of adjoints, which typically increase with the increase in the number of model parameters and the sought order of variation. EpGPT however calculates a small number of adjoint functions corresponding to a small number of pseudo responses which represent randomized linear combinations of the flux values everywhere in the phase space. The resulting adjoints can be used to be used to analytically combine all higher order variations to a given preset tolerance for a general parameter perturbation. If the parameter perturbations are small, one can extract first-order sensitivities like GPT. With large perturbations however, one can use the resulting EpGPT analytical expression as a surrogate model for the original transport model. Previous work has demonstrated that EpGPT can be used to evaluate the variations in neutron flux and responses of interest due to various perturbations, such as cross sections, fuel enrichment, fuel densities, temperatures, etc., in lattice design calculations. We briefly discuss the EpGPT approach, and refer the reader to Ref. [2] for detailed description.

The steady-state linear Boltzmann equation describing neutron transport can be represented in operator form by eigenvalue equation,

$$\mathbf{P}\phi = (\mathbf{L} - \lambda\mathbf{F})\phi = 0 \quad (1)$$

where  $\lambda = 1/k$ , and  $\phi \in \mathbb{R}^n$  is the neutron angular flux. The scattering and differential transport operators are represented by  $\mathbf{L}$  and the fission transport operator by  $\mathbf{F}$ . In the following, we refer to the operator  $\mathbf{P} = (\mathbf{L} - \lambda\mathbf{F})$  as the transport operator. The neutron flux is normalized as follows:

$$\langle h, \phi \rangle = 1 \quad (2)$$

Assume that all possible state variations  $\Delta\phi$  belong to a subspace  $\mathbb{Z}$  of size  $r$

$$\Delta\phi = \beta_1 q_1 + \beta_2 q_2 + \dots + \beta_r q_r = \sum_{i=1}^r \beta_i q_i; \text{ with } \Delta\phi \in \mathbb{R}^n, q_i \in \mathbb{R}^n, \beta_i \in \mathbb{R}^r \quad (3)$$

where  $q_i$  represents an orthonormal basis vector function in the discretized scheme in the subspace  $\mathbb{Z}$ . If  $r$  is much smaller than  $n$  (the size of the state space), one can recast GPT in terms of a set of  $r$  pseudo responses. In doing so, one recognizes that the remaining  $n-r$  directions in the flux space have negligible impact on the response. As shown in Ref. [2], the coefficient vector  $\beta = [\beta_1, \dots, \beta_r]^T$  is equal to:

$$\beta = -(\mathbf{I} + \mathbf{T})^{-1} \varpi \quad (4)$$

with

$$\varpi = \left[ \langle \Gamma_1^*, \Delta\mathbf{P}\phi_0 \rangle \quad \dots \quad \langle \Gamma_r^*, \Delta\mathbf{P}\phi_0 \rangle \right]^T$$

$$\mathbf{T} = \begin{bmatrix} \langle \Gamma_1^*, \Delta\mathbf{P}q_1 \rangle & \dots & \langle \Gamma_1^*, \Delta\mathbf{P}q_j \rangle & \dots & \langle \Gamma_1^*, \Delta\mathbf{P}q_r \rangle \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \langle \Gamma_i^*, \Delta\mathbf{P}q_1 \rangle & \dots & \langle \Gamma_i^*, \Delta\mathbf{P}q_j \rangle & \dots & \langle \Gamma_i^*, \Delta\mathbf{P}q_r \rangle \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \langle \Gamma_r^*, \Delta\mathbf{P}q_1 \rangle & \dots & \langle \Gamma_r^*, \Delta\mathbf{P}q_j \rangle & \dots & \langle \Gamma_r^*, \Delta\mathbf{P}q_r \rangle \end{bmatrix} \in \mathbb{R}^{r \times r}$$

where  $\mathbf{I}$  is  $r$  by  $r$  identity matrix, and the perturbed neutron transport operator  $\Delta\mathbf{P} = (\Delta\mathbf{L} - \lambda\Delta\mathbf{F} - \Delta\lambda\mathbf{F} - \Delta\lambda\Delta\mathbf{F})$ . The functions  $\{\Gamma_i^*\}_{i=1}^r$  are the generalized adjoint fluxes, which are the solutions to the generalized adjoint transport equation:

$$\mathbf{P}^* \Gamma_i^* = \frac{\partial R_i}{\partial \phi} = q_i - N_i^* h, \text{ for } i = 1, \dots, r \quad (5)$$

where  $R_i = \langle q_i, \phi \rangle$ , for  $i = 1, \dots, r$  is the pseudo response used to capture the flux variations, and  $\mathbf{P}^*$  is adjoint operator to the forward transport operator. Considering the source provided in Eq. (5) is orthogonal to the forward flux, i.e.

$$\langle (q_i - N_i^* h), \phi \rangle = 0, \text{ for } i = 1, \dots, r \quad (6)$$

thus, one can choose  $N_i^* = \frac{\langle q_i, \phi \rangle}{\langle h, \phi \rangle}$ , for  $i = 1, \dots, r$ .

This derivation shows that adjoint formulation of EPGPT is very similar to standard GPT with the exception of the different source formulation for the GPT equation. This implies that the EPGPT surrogate can be easily implemented in other computer codes which have a GPT capability.

## 2.2 Subspace-based Uncertainty Quantification

A basic ingredient in the ROM algorithm is the capability to perturb the model parameters (refers here to the multi-group cross-sections). ROM methods require two different modes for cross-section perturbations. An initial purely random perturbation of all cross-sections to identify the active subspace, followed by a selective perturbation approach which employs the results of the first set of code runs to either construct a surrogate model of identify the dominant directions for a subsequent subspace-based UQ. This requires a capability to introduce user-defined perturbations which is currently not available in the SAMPLER super-sequence. The SAMPLER generates cross-section perturbations that are consistent with the multi-group cross-section covariance matrix using the XSUSA methodology<sup>3</sup>. We therefore modify the SAMPLER perturbation routines to allow introduction of random and user-defined perturbations as required by the ROM application.

Consider a mathematical model described by the following equation:

$$y = f(x) \quad (7)$$

where  $x \in R^n$  denotes the  $n$ -component vector for input parameters, and  $y \in R^m$  represents the  $m$  model's responses of interest. As discussed in the literature, one can employ the adjoint-based perturbation theory to calculate the sensitivity coefficients for given response with respect to all input parameters<sup>8</sup>, i.e.

$$[\mathbf{S}]_{ij} = \frac{\partial y_i}{\partial x_j}, \text{ for } i = 1, \dots, m, j = 1, \dots, n \quad (8)$$

where  $\mathbf{S}$  is denoted as the sensitivity matrix. The row space of  $\mathbf{S}$ , denoted by  $R(\mathbf{S}^T)$  or S-subspace, can be employed to construct an active subspace that can be used for input parameters space reduction. The size of the active subspace is determined by the effective rank of the matrix  $\mathbf{S}$ , which can be obtained by RFAs.

In our current implementation, the input parameters represent the nuclear cross sections whose uncertainties are characterized by a covariance matrix  $\mathbf{C}_x \in R^{n \times n}$ . The covariance matrix is a symmetric positive semi-definite matrix with diagonal entries representing the variance of the cross-sections, and off-diagonal entries representing the correlations therein. RFAs can also be used to identify the active subspace for  $R(\mathbf{C}_x)$ , denoted hereinafter as C-subspace. The C-subspace identifies directions in the parameter space associated with high uncertainties.

CRANE employs RFAs to identify a third subspace, referred to as the intersection subspace, which captures directions in the parameter space that are associated with a high net product of sensitivities and uncertainties. This is done via adjoint-based perturbation theory to compute the sensitivity coefficients of pseudo responses. A pseudo response is an abstraction that allows one generate randomized linear combination of the various model's responses sensitivity profiles. For example, a pseudo response for the model represented by Eq. (7) can be defined as:

$$y_{pseudo} = \theta^T y$$

where  $y \in R^m$  represents the  $m$  model's responses of interest, and  $\theta$  is a random vector.

In current CRANE implementation, the sampling of nuclear data is accomplished in the following steps:

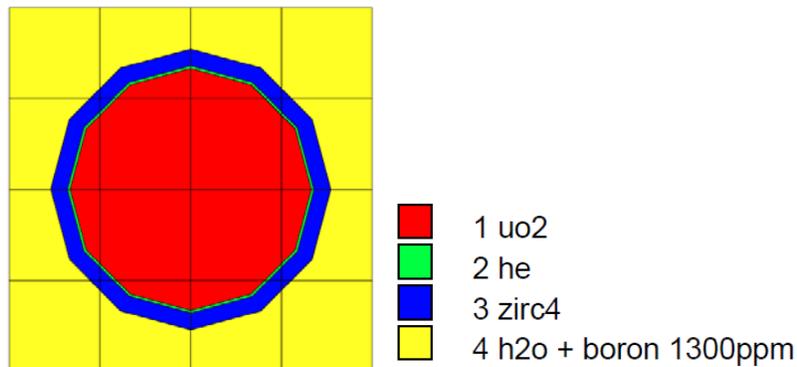
1. Generate  $l$  random vectors  $\theta_i \Big|_{i=1}^l \in R^m$ ;
2. Construct  $l$  pseudo responses:  $Y_{i,pseudo} = \theta_i^T y \Big|_{i=1}^l$ ;
3. Compute  $\frac{dY_{i,pseudo}}{dx} \Big|_{i=1}^l$  via adjoint-based perturbation theory;
4. SVD decomposition for covariance matrix:  $\mathbf{C}_x = \mathbf{U}_x \Sigma_x \mathbf{U}_x^T$ ;
5. Calculate  $\mathbf{G} = \Sigma_x^{1/2} \mathbf{U}_x^T \left[ \frac{dY_{1,pseudo}}{dx}, \dots, \frac{dY_{l,pseudo}}{dx} \right] \in R^{n \times l}$
6. Determine the "intersection" subspace via orthogonal decomposition of  $\mathbf{G} = \mathbf{Q}\mathbf{R}$ , where  $\mathbf{Q} = [q_1, \dots, q_l]$ ;
7. Employ RFA algorithm to identify the effective rank  $r$  of matrix  $\mathbf{Q}$ ;

8. Using  $\kappa$ -metric<sup>6</sup> to examine the reduction errors, if the error tolerance criterion is not met, increase  $l$  and go back to step 1;
9. Generate  $N$  random vectors using standard norm distribution:  $w_i \in R^T$ ,  $i = 1, \dots, N$ ;
10. Construct  $N$  parameter perturbation of the form:  $\Delta x_i = U_x \Sigma_x^{1/2} Q w_i$ ,  $i = 1, 2, \dots, N$ ;
11. Run SAMPLER with the determined  $N$  perturbations
12. Statistically analyze the results for estimating mean and standard deviation.

In step 11, we employ SAMPLER to propagate the uncertainties, this is because SAMPLER is able to explicitly treat resonance self-shielding effects. As can be observed, both SAMPLER and CRANE randomly sample the parameters, and calculate statistics on the response variations. The difference is that the purely random sampling approach in SAMPLER is guided only the prior covariance matrix, however the approach implemented in CRANE confines the samples to an active subspace that contains the key contributors to uncertainties. This is not possible with a forward sampling approach unless the number of samples is taken to be at least as large as the number of parameters, which is impractical for neutronics models.

### 3. NUMERICAL RESULTS

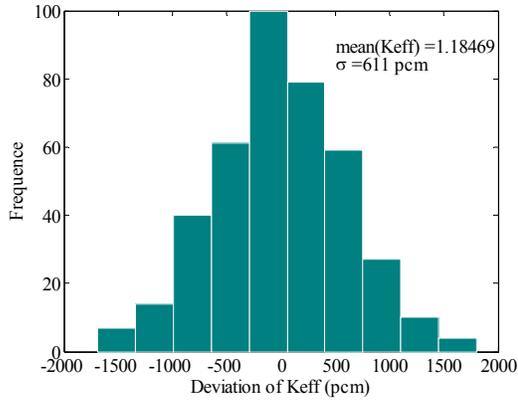
A 2D PWR pin-cell model, referred to as progression problem 1a of a standard CASL suite for neutronics models testing, is employed here to demonstrate the functionality of CRANE. The pin-cell is based on a 17x17 Westinghouse standard PWR assembly model. The materials included in the pin-cell model are  $UO_2$ , zircaloy-4, and water. The moderator contains soluble boron as a chemical shim for maintaining criticality, and the pellet-clad gap contains helium gas. This problem represents typical zero power isothermal conditions which are representative of power reactor startup physics testing. The model layout is shown in Fig. 1. The SCALE6.2B2 code package is employed<sup>9</sup>.



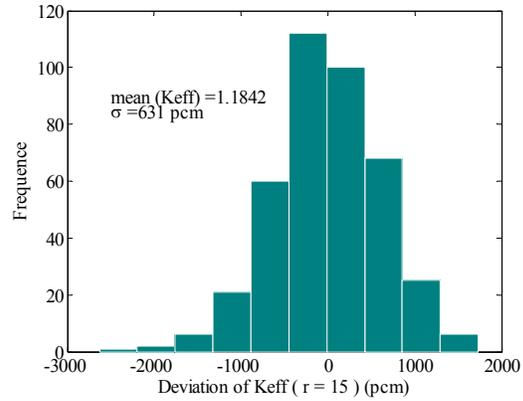
**Fig. 1.** Model Layout

The cross sections, i.e. scattering, radiation capture, fission, etc., are randomly perturbed using CRANE to identify the active subspace. CRANE is then employed to propagate the uncertainties via intersection subspace UQ method. The nominal dimension of input parameter space is 11,308. Fig. 2-b plots the histogram of  $K_{eff}$  variations due to

cross section perturbations confined to the active intersection subspace with size of 15, i.e., implying only 15 dominant directions, while the reference Keff is obtained by computing the mean value of all perturbed cases. For comparison, Fig. 2-a plots the histogram of Keff variations generated via SAMPLER using the standard XSUSA approach. In addition, for comparison purposes, the TSUNAMI-2D was employed to compute the standard derivation of Keff, i.e.  $\sigma(K_{eff}) = 625.1 pcm$ , via first-order generalized perturbation theory.



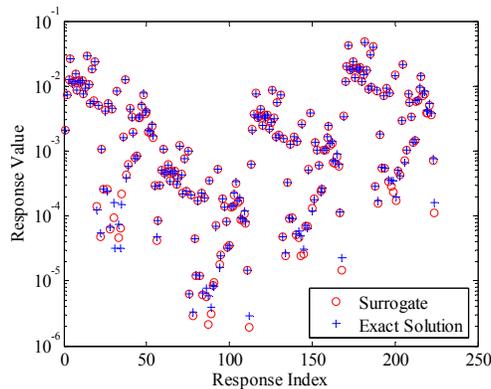
**Fig. 2-a.** Histogram of Keff Variations via SAMPLER



**Fig. 2-b.** Histogram of Keff Variations via CRANE

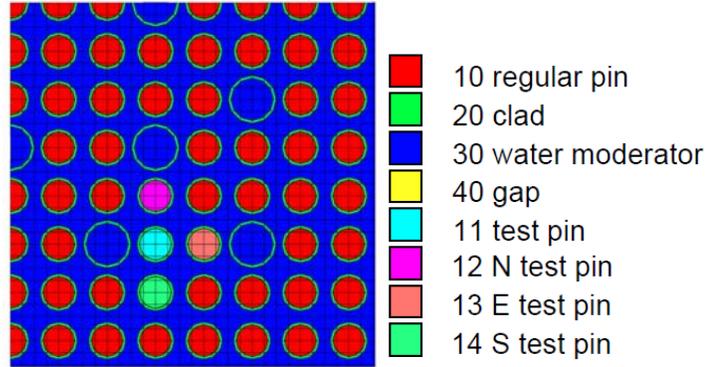
**Fig. 2.** Comparison between CRANE and SAMPLER

The previous model was employed to demonstrate the  $E_P$ GPT functionality of CRANE. The nominal dimension of neutron flux space is 157,248. The sizes of the parameters and flux active subspaces are 200 and 100, respectively. For a given random perturbation (Fig. 3), the variation in the eigenvalue is 13,952 pcm, while the discrepancies in the eigenvalue predictions is 78.5 pcm. The discrepancies in the eigenvalue prediction between first-order GPT and the direct neutron transport calculations is 1107.9 pcm. Fig. 3 shows the values of 224 different responses of interest, i.e. group-wised mixture flux, computed by  $E_P$ GPT surrogate model and NEWT model, respectively.



**Fig. 3.** Response Approximation via  $E_P$ GPT Surrogate

An assembly model was also used to demonstrate application of EpGPT. This model layout, a UO<sub>2</sub> Gösgen (ARIANE) sample<sup>11</sup>, is shown in Fig. 4. The specific enrichments for each of the pin types may be found in Ref. [11].

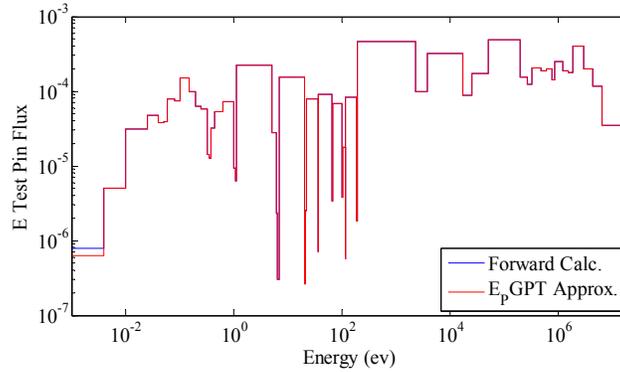


**Fig. 4.** Assembly model layout

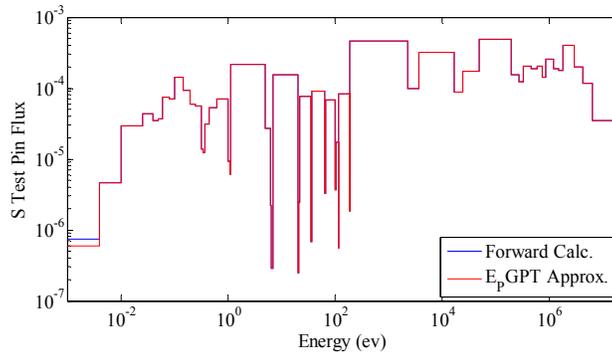
The standard SCALE 56-group cross section library (xn56v7 generated from ENDF/B-VII.0 64-group neutron library) is employed. The dimension of the angular flux is 3,929,856 (i.e. angular quadrature  $S_N=6$ , 56 energy groups and 2924 cells). The flux predicted by the EpGPT surrogate, using a subspace with size 60, are compared to the exact fluxes predicted by NEWT<sup>10</sup>. We will refer to  $\|\phi_{Exact} - \phi_{EPGPT}\|_2 / \|\phi_{Exact}\|_2$  as the relative error in the flux. Large number of randomized cross-section perturbations, giving rise to 1% change in reactivity, were used to assess the quality of EpGPT surrogate predictions. Specifically, the upper bounds on the flux errors are:

$$\frac{\|\phi_{Exact} - \phi_{EPGPT}\|_2}{\|\phi_{Exact}\|_2} = 5.73E - 4$$

The corresponding upper-bound on the  $K_{eff}$  is found to be 0.0047%, or approximately 5pcm. In practice, one could employ higher size for the active subspace if higher accuracy is required. A small value is used here to demonstrate that reasonable accuracy can be obtained with very small active subspace as compared to the original flux space. Figs. 5 and 6 show the flux spectra for fuel in two types of pins, the E test pin, and the S test pin as shown in Fig. 4.



**Fig. 5. Flux spectrum for the E test pins**



**Fig. 6. Flux spectrum for the S test pins**

#### 4. CONCLUSIONS

The recently developed CRANE super-sequence has been equipped with a number of functionalities to support the efficient execution of uncertainty quantification and the construction of accuracy-preserving surrogate models. Both functionalities are currently fully automated in CRANE and are ready for release to interested beta users. Future work will focus on further customization of the tool for specific applications, e.g., generation of few-group cross-sections for downstream core-wide calculations.

#### ACKNOWLEDGMENTS

This work was supported by the School of Nuclear Engineering at Purdue University.

## REFERENCES

1. C. Wang, J. Hite and H. S. Abdel-Khalik, "Intersection Subspace Method for Uncertainty Quantification," *Transactions of the American Nuclear Society*, **111**, pp.1384-1387 (2014).
2. C. Wang and H. S. Abdel-Khalik, "Exact-to-Precision Generalized Perturbation Theory for Neutron Transport Calculation," *Proceedings of the 2013 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Sun Valley, Idaho, May 5-9, **45**, pp. 828-841 (2013)
3. M. L. Williams, et al., "A Statistical Sampling Method for Uncertainty Analysis with SCALE and XSUSA," *Nuclear Technology*, **183**, pp. 515-526 (2013).
4. B. O. Almroth, F. A. Brogan and P. Stern, "Automatic choice of global shape functions in structural analysis," *AIAA Journal*, **16**, pp. 525-528 (1978).
5. G. Rozza, "Reduced Basis Approximation and Error Bounds for Potential Flows in Parameterized Geometries," *Communication in Computational Physics*, **9**, pp. 1-48 (2011).
6. M. G. Abdo and H. S. Abdel-Khalik, "Probabilistic Error Bounds for Reduced Order Modeling," MC2015, Nashville, TN 2015
7. H. S. Abdel-Khalik, Tutorial Series on Characterization of Uncertainty (TUSC): Reduced Order Modeling, Dimensionality Reduction, Surrogate Modeling, Function Approximation, Fitting, etc.", ANFM2015, Hilton Head, SC 2015
8. C. Wang and H. S. Abdel-Khalik, "Accuracy Preserving Surrogate for Neutron Transport Calculations," *Proceeding of PHYSOR 2014*, The Westin Miyako, Kyoto, Japan, Sept. 28 – Oct. 3 (2014).
9. M. L. Williams, *Perturbation Theory for Reactor Analysis*, CRC Handbook of Nuclear Reactor Calculations, CRC Press (1986).
10. *Scale: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design*, ORNL/TM-2005/39, Version 6.1, Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785, Oak Ridge, TN (RSICC 2011).
11. G. Radulescu, I. C. Gauld and G. Ilas, "SCALE 5.1 Predictions of PWR Spent Nuclear Fuel Isotopic Compositions," Nuclear Science and Technology Division, ORNL/TM-2010/44 (2010).