A New SCALE Capability for Uncertainty Quantification of Kinetic Parameters

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Content

- **Background**
- The Framework Description
- Preliminary Analysis
- Applications
  - Sensitivity Analysis
  - Reduced Order Modeling (ROM)
  - ROM-based UQ
  - Variance Decomposition by Sobol indices
- Summary

Background

- Delayed neutrons are important for reactor control as they make the nuclear reactor controllable.
- Importance of kinetic parameters' uncertainty to the reactor modeling.
- The conventional kinetics model is to divide the delayed neutron precursors into six groups (i.e. N=6).
- For core calculations, homogenized kinetic parameters (β_{eff}, β_i, λ_i, λ_{eff}) averaged over all isotopes are needed along with their uncertainty.
- At the end, you provide a single value of each kinetic parameter (e.g. β_{eff}) which represents the average of all delayed neutron emitters.
- The sources of uncertainty:

1. Fundamental Nuclear Data: XS (e.g., ν, Σ_f, χ)
2. Fundamental Delayed Neutron Data: DND (e.g. $a_{j,i}$, $\lambda_{j,i}$)

$$\frac{dn(t)}{dt} = \frac{\rho - \boxed{\beta_{eff}}}{\Lambda} n(t) + \sum_{i=1}^{N} \boxed{\lambda_i} C_i(t)$$

$$\frac{dC_i(t)}{dt} = \frac{\boxed{\beta_i}}{\Lambda} n(t) - \boxed{\lambda_i} C_i(t), \qquad (i = 1, \ldots, N)$$

Response of Interest (Homogenized Kinetic Parameters):

$$\beta_{j,i} = a_{j,i} Y_j$$

$$\beta_i = \frac{\sum_j \beta_{j,i} \sum_m \sum_g \bar{\nu}\Sigma_f^{j,m,g} \ \varphi_{m,g} V_m \ \sum_{g'} \chi_d^{g',i} \varphi_{g'}^*}{\sum_j \sum_m \sum_g \bar{\nu}\Sigma_f^{j,m,g} \ \varphi_{m,g} V_m \sum_{g'} \chi^{g'} \varphi_{g'}^*}$$

$$\lambda_i = \frac{\sum_j \lambda_{j,i} \ \beta_{j,i} \sum_m \sum_g \bar{\nu}\Sigma_f^{j,m,g} \ \varphi_{m,g} V_m}{\beta_i \sum_j \sum_m \sum_g \bar{\nu}\Sigma_f^{j,m,g} \ \varphi_{m,g} V_m}$$

$$\beta_{eff} = \sum_{i=1}^{N} \beta_i \qquad\qquad \lambda_{eff} = \frac{\beta_{eff}}{\sum_{i=1}^{N} \frac{\beta_i}{\lambda_i}}$$

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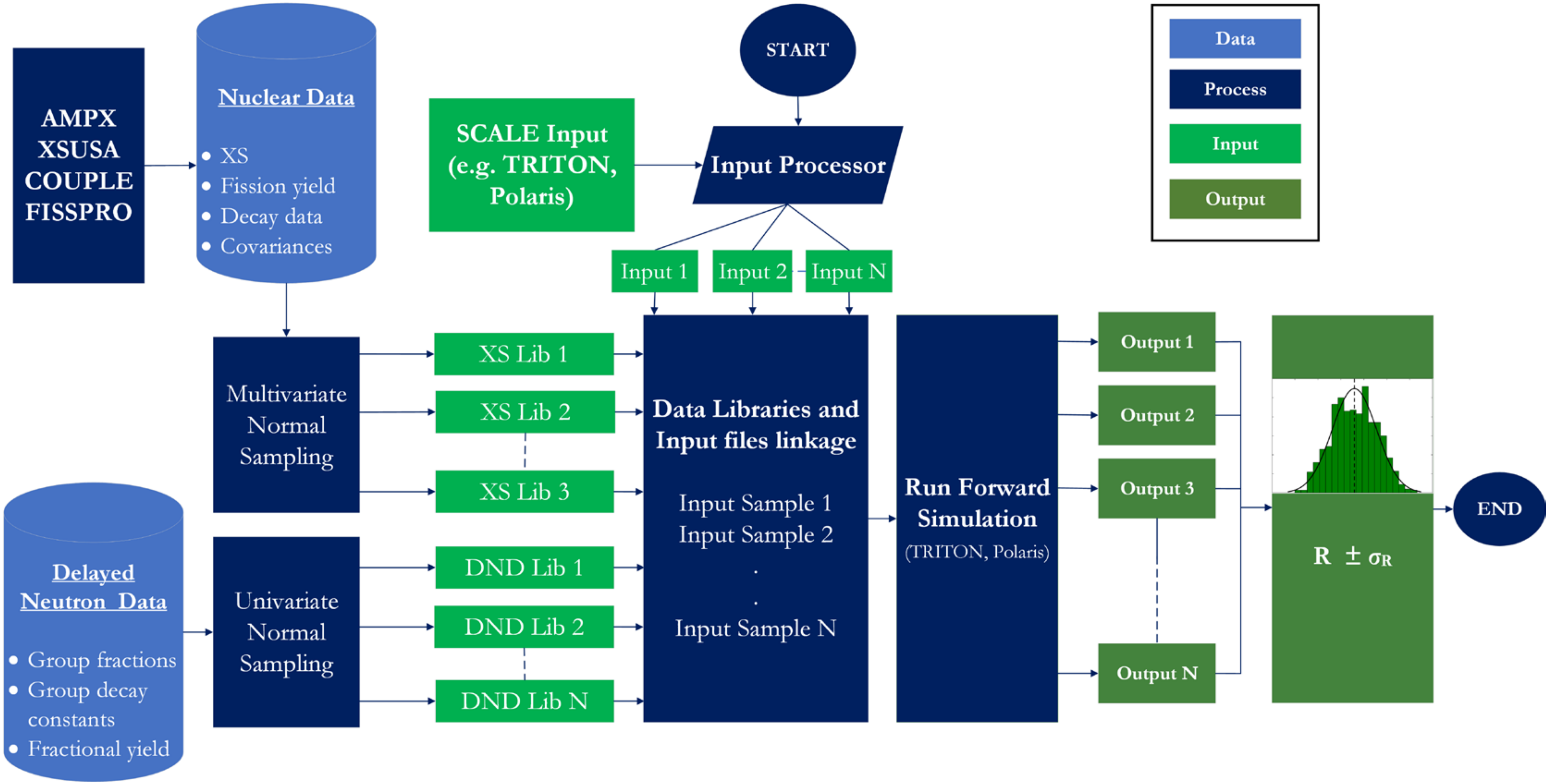
SCALE/Sampler with DND



Delayed Neutron Data

- Fundamental delayed neutron parameters: $a_{j,i}, \lambda_{j,i}, Y_{,i}$.
- The notation for delayed neutron data

$X_{i,g}^{Isotope}$

Where:
$X = a, \lambda, Y$ (Parameter)
Isotope: U235, U238, etc.
$i = 1, 2, .., 6$ (Precursor group)
$g = 1, 2$ (Energy group)

- Examples:

$a_{3,2}^{U235}$

$\lambda_{2,1}^{U238}$

Table 1: Measured delayed neutron group parameters for the isotopes whose both thermal and fast sets

Isotope	No.	$a_{i,j}$ (F[a])	$\lambda_{i,j}$ (F)	$a_{i,j}$ (T[a])	$\lambda_{i,j}$ (T)	Source
U-233	1	0.086 ± 0.004	0.0126 ± 0.0006	0.086 ± 0.003	0.0126 ± 0.0001	F: Tuttle (1975)
	2	0.274 ± 0.007	0.0334 ± 0.0021	0.299 ± 0.004	0.0337 ± 0.0006	T: Keepin et al. (1957)
	3	0.227 ± 0.052	0.1310 ± 0.0070	0.252 ± 0.040	0.1386 ± 0.0058	
	4	0.317 ± 0.016	0.3020 ± 0.0360	0.278 ± 0.020	0.3254 ± 0.0306	
	5	0.073 ± 0.021	1.2700 ± 0.3900	0.051 ± 0.024	1.1271 ± 0.4435	
	6	0.023 ± 0.010	3.1300 ± 1.0000	0.034 ± 0.014	2.5023 ± 0.4246	
U-235	1	0.038 ± 0.004	0.0127 ± 0.0003	0.033 ± 0.003	0.0124 ± 0.0003	F: Tuttle (1975)
	2	0.213 ± 0.007	0.0317 ± 0.0012	0.219 ± 0.009	0.0305 ± 0.0010	T: Keepin et al. (1957)
	3	0.188 ± 0.024	0.1150 ± 0.0040	0.196 ± 0.022	0.1114 ± 0.0041	
	4	0.407 ± 0.010	0.3110 ± 0.0120	0.395 ± 0.011	0.3014 ± 0.0118	
	5	0.128 ± 0.012	1.4000 ± 0.1200	0.115 ± 0.009	1.1363 ± 0.1546	
	6	0.026 ± 0.004	3.8700 ± 0.5500	0.042 ± 0.008	3.0137 ± 0.3276	
Pu-239	1	0.038 ± 0.004	0.0129 ± 0.0003	0.035 ± 0.009	0.0128 ± 0.0006	F: Tuttle (1975)
	2	0.280 ± 0.006	0.0311 ± 0.0007	0.298 ± 0.035	0.0301 ± 0.0022	T: Keepin et al. (1957)
	3	0.216 ± 0.027	0.1340 ± 0.0040	0.211 ± 0.048	0.1238 ± 0.0088	
	4	0.328 ± 0.015	0.3310 ± 0.0180	0.326 ± 0.033	0.3254 ± 0.0367	
	5	0.103 ± 0.013	1.2600 ± 0.1700	0.086 ± 0.029	1.1216 ± 0.3866	
	6	0.035 ± 0.007	3.2100 ± 0.3800	0.044 ± 0.016	2.6971 ± 0.4722	

[a] In this table: F refers to fast fission and T refers to thermal fission.

[1] Keepin, G. R., Wimett, T. F., & Zeigler, R. K. (1957). Delayed neutrons from fissionable isotopes of uranium, plutonium, and thorium. Physical review, 107(4), 1044.
[2] Tuttle, R. J. (1975). Delayed-neutron data for reactor-physics analysis. Nuclear Science and Engineering, 56(1), 37-71.

Delayed Neutron Data

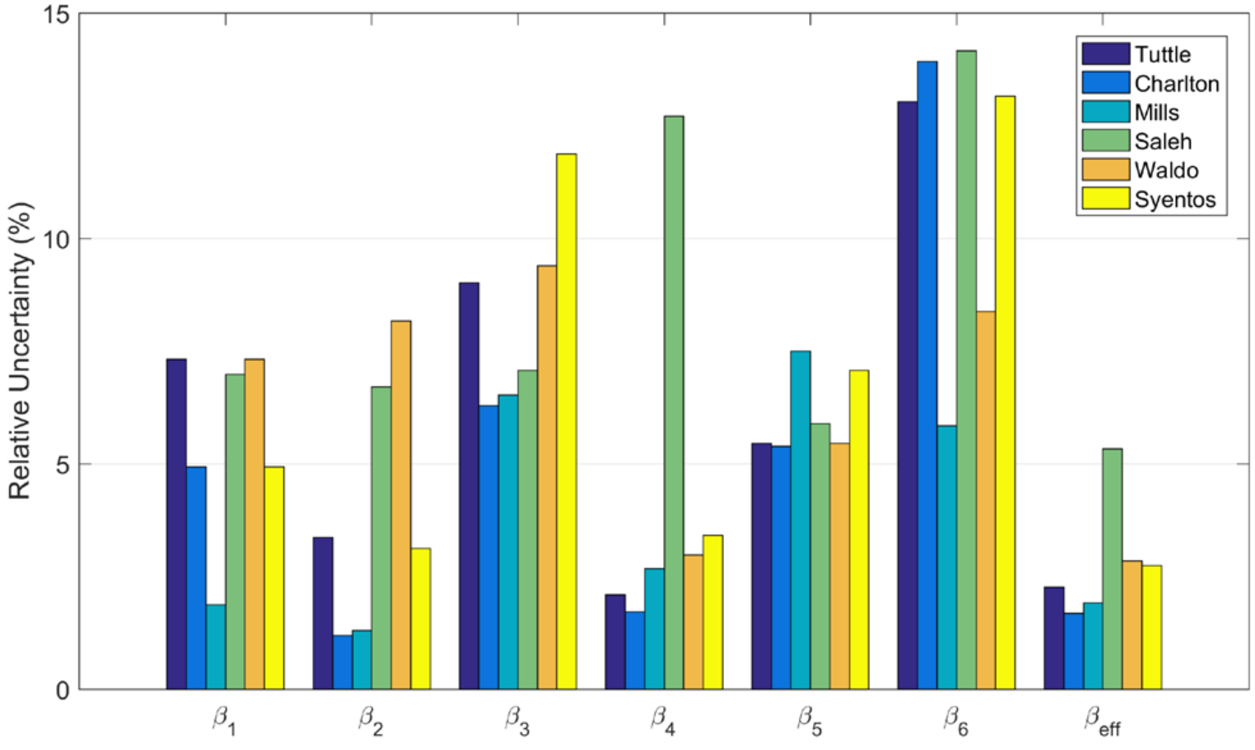
Table 2: Measured values of absolute delayed neutron yield ($\bar{\nu}_d$) for the selected actinides plus uncertainty collected from different sources

isotope	$\bar{\nu}_d$ (F)	Source	$\bar{\nu}_d$ (T)	Source
Th-227	-	-	0.00769 ± 0.00115	SCALE Rearden and Jessee (2018)
Th-229	-	-	0.01621 ± 0.00243	SCALE Rearden and Jessee (2018)
Th-232	0.05470 ± 0.00120	Tuttle (1975)	-	-
Pa-231	0.01110 ± 0.00110	Wilson and England (2002)	-	-
U-232	-	-	0.00437 ± 0.00033	Waldo et al. (1981)
U-233	0.00729 ± 0.00019	Tuttle (1975)	0.00664 ± 0.00018	Tuttle (1975)
U-234	0.01060 ± 0.00120	Tuttle (1975)	-	-
U-235	0.01650 ± 0.00075	Keepin (1965)	0.01580 ± 0.00075	Keepin (1965)
U-236	0.02310 ± 0.00260	Tuttle (1975)	-	-
U-238	0.04510 ± 0.00061	Tuttle (1975)	-	-
Np-237	0.01260 ± 0.00070	Saleh et al. (1997)	0.01290 ± 0.00040	Loaiza et al. (1998)
Pu-238	0.00461 ± 0.00073	Waldo et al. (1981)	-	-
Pu-239	0.00664 ± 0.00013	Tuttle (1975)	0.00624 ± 0.00024	Tuttle (1975)
Pu-240	0.00960 ± 0.00110	Tuttle (1975)	-	-
Pu-241	0.01630 ± 0.00160	Tuttle (1975)	0.01560 ± 0.00160	Tuttle (1975)
Pu-242	0.02280 ± 0.00250	Tuttle (1975)	-	-
Am-241	-	-	0.00490 ± 0.00020	Saleh et al. (1997)
Am-243	0.00860 ± 0.00050	Charlton et al. (1997)	0.00800 ± 0.00040	Saleh et al. (1997)
Cm-245	-	-	0.00592 ± 0.00039	Waldo et al. (1981)
Cf-252*	0.00812 ± 0.00053	Wahl (1988)	-	-

*The data for Cf-252 is the delayed neutron yield resulted form spontaneous fission.

Delayed Neutron Data (Selection Criteria)

- In general, the group parameters and absolute yield for most of the fast fission data were taken from Tuttle (1975) due to their high accuracy.
- The group parameters and absolute yield for thermal fission data of U-233, U-235, and Pu-239 were taken from Keepin et al. (1957). Indeed, Tuttle (1975) suggested using Keepin data for thermal fission on the basis of higher quality.
- It is preferred to use the absolute delayed neutron yield from the same study as the group parameters, since the group fractions are calculated (normalized) using the measured delayed neutron yield.
- If the isotope data is … urce is used for the group parameters and …
- If there is no experim … ıputational-based data was selected from Wil … l hence had no effect on the UQ results.
- If there is no experim … eutron experiments, the value and its uncertair … l on ENDF-B/VII.1.
- All nubar and its uncer … ısed on ENDF-B/VII.1.
- Exceptions to the previ … he text.



The Framework Features

DND: Delayed Neutron Data

Supports fundamental delayed neutron data for 20 actinides based on various delayed neutron experiments.

Because of lack of reliable correlation matrices for the delayed neutron data, the framework supports uncorrelated DND.

The user can replace those libraries easily with other libraries sampled using different methods or for point-wise sensitivity analysis.

The base DND data libraries “kinetics.dat”, “kinetics_var.dat” can be changed easily to account for new isotopes or other DND data sources.

The framework can be activated easily using the option “perturb_kinetics” in Sampler.

The framework supports kinetics UQ in TRITON and Polaris Sequences in SCALE.

The framework is expected to be a part of Sampler in SCALE-6.3 version.

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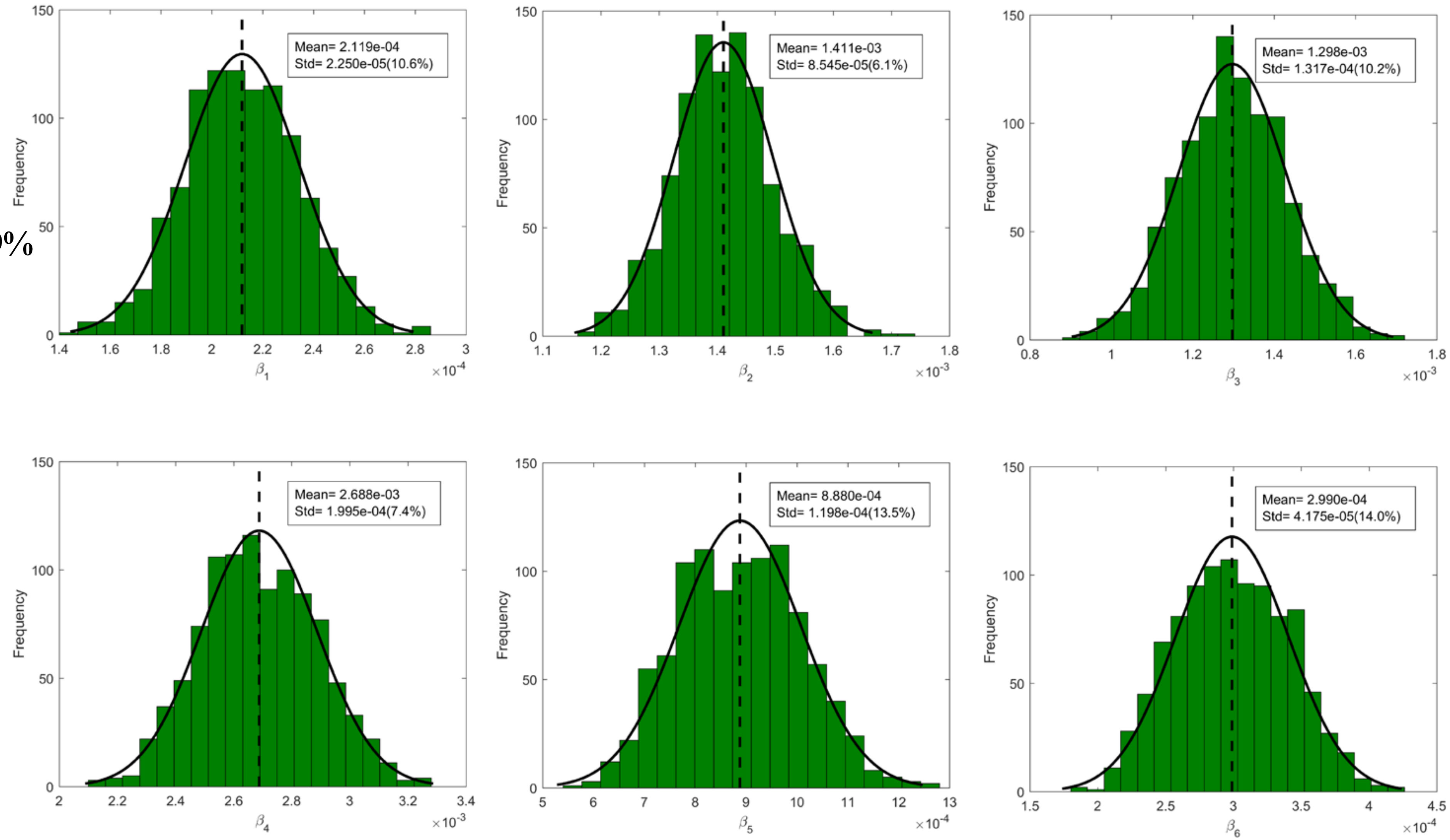
Group-Wise Beta Uncertainty (β_i)

- Note: the spread is caused by uncertainties in DND and XS

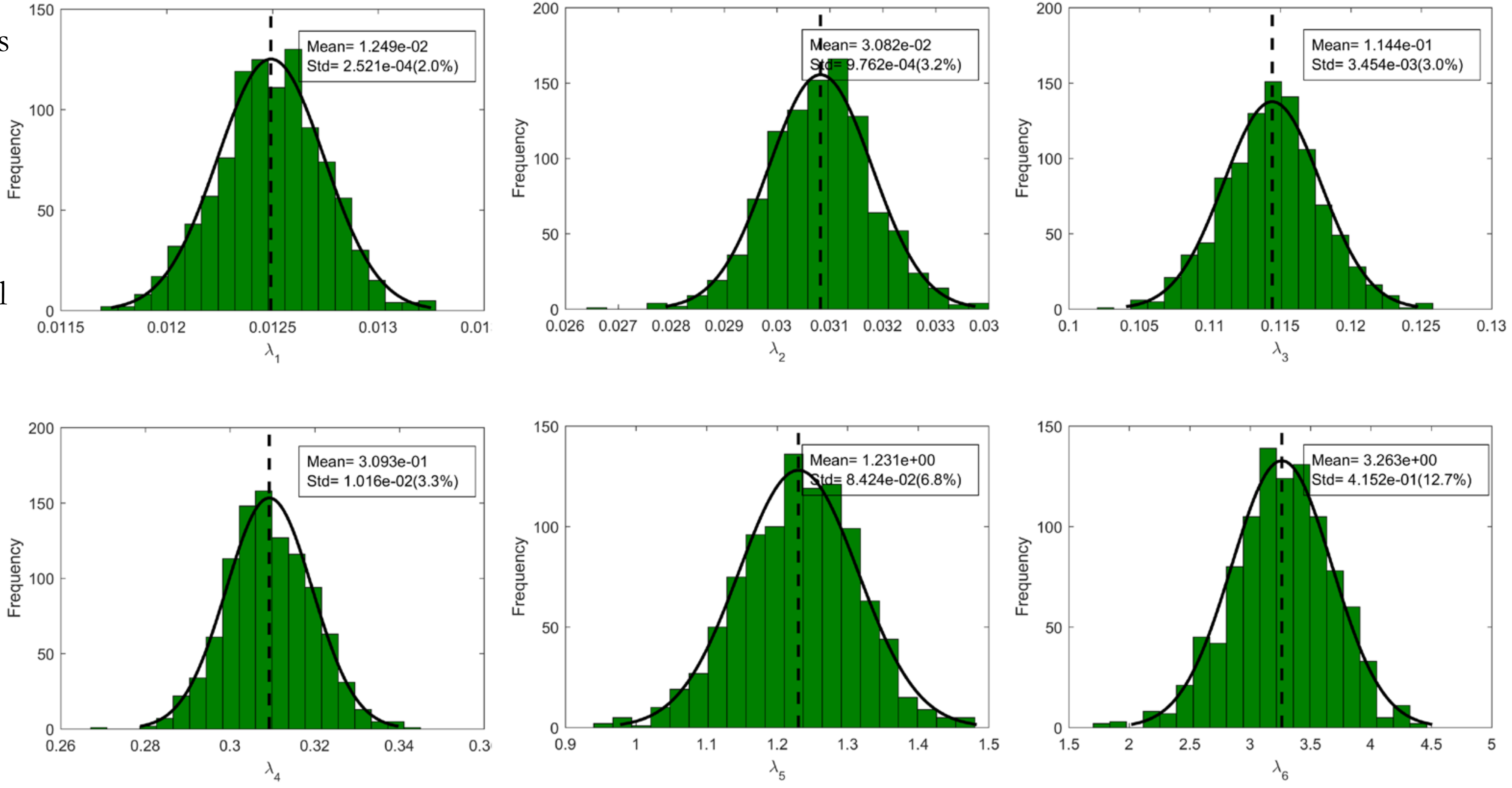
β_{eff} uncertainty ~ 7-9%

- Calculations were based on a pin-cell geometry from UAM benchmark



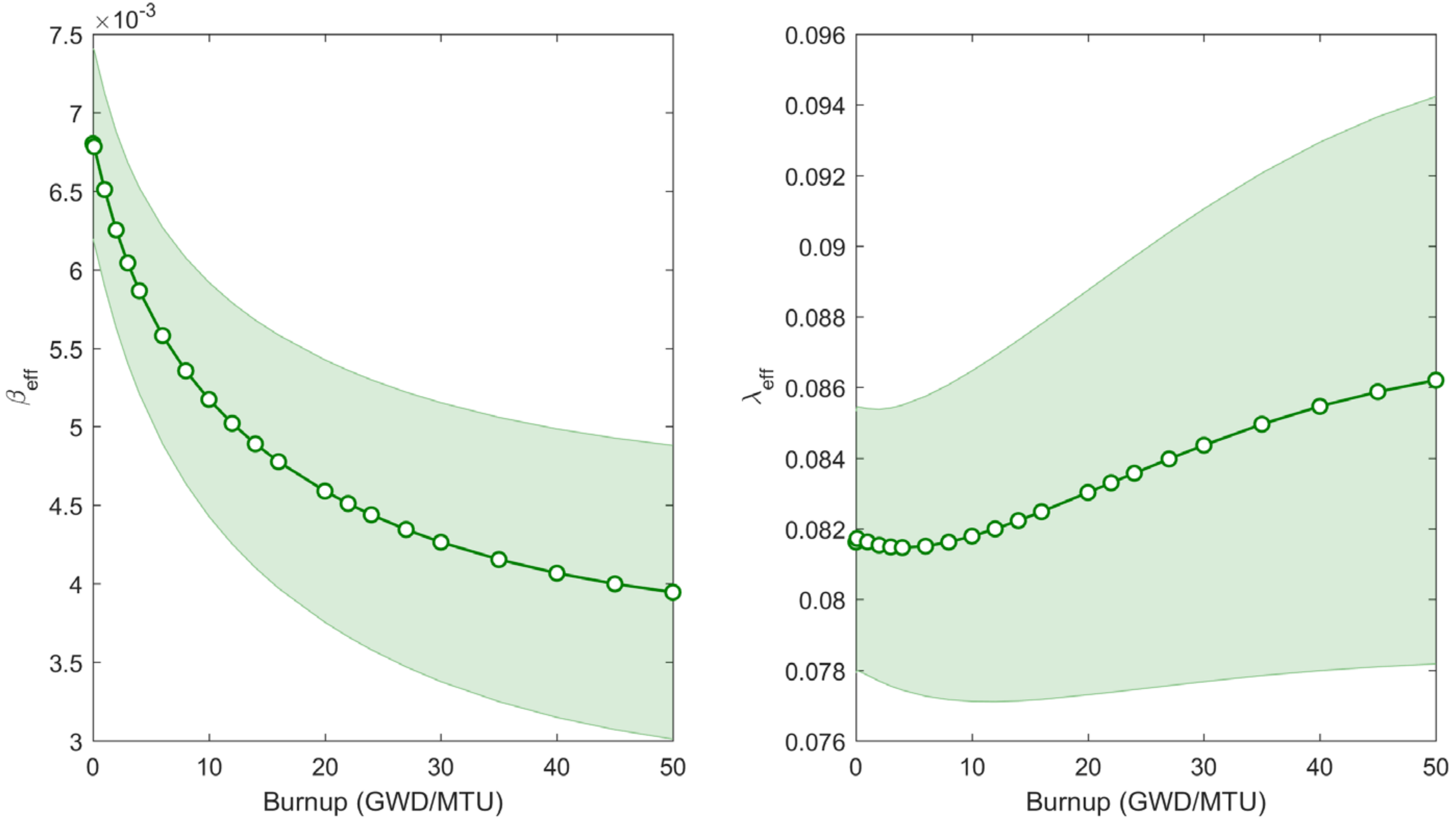
Group-Wise Lambda Uncertainty (λ_i)

- Note: the spread is caused by uncertainties in DND and XS
- Calculations were based on a pin-cell geometry from UAM benchmark

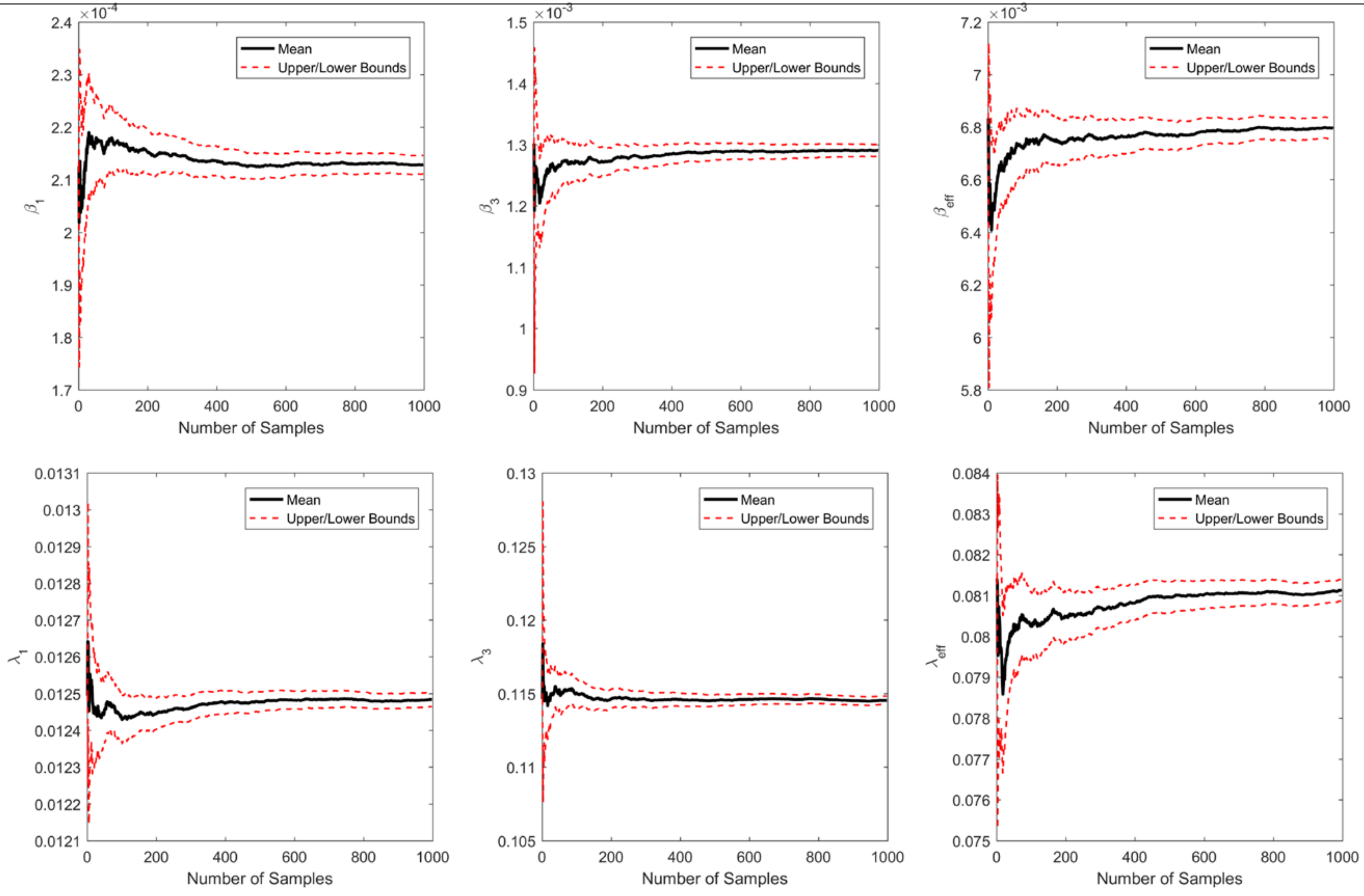


Burnup-dependent Kinetic Parameters

Notes:
- The spread is caused by uncertainties in DND and XS
- The error bar is ±1σ around the mean



Convergence Analysis



TRITON vs Polaris

Table 6: Comparison of the kinetic parameters' value and uncertainty between TRITON and Polaris lattice physics codes for a PWR pin-cell

Parameter	TRITON			Polaris		
	Mean	Std	Relative(%)	Mean	Std	Relative(%)
β_1	2.112E-04	1.755E-05	8.3	2.124E-04	1.716E-05	8.1
β_2	1.412E-03	8.752E-05	6.2	1.415E-03	9.422E-05	6.7
β_3	1.291E-03	1.432E-04	11.1	1.299E-03	1.457E-04	11.2
β_4	2.689E-03	1.992E-04	7.4	2.725E-03	2.275E-04	8.3
β_5	8.882E-04	1.131E-04	12.7	9.197E-04	1.299E-04	14.1
β_6	2.988E-04	5.305E-05	17.8	3.020E-04	5.516E-05	18.3
β_{eff}	6.790E-03	5.064E-04	7.5	6.873E-03	5.785E-04	8.4
λ_1	1.249E-02	2.411E-04	1.9	1.252E-02	2.263E-04	1.8
λ_2	3.081E-02	7.982E-04	2.6	3.089E-02	7.525E-04	2.4
λ_3	1.148E-01	3.572E-03	3.1	1.155E-01	3.511E-03	3.0
λ_4	3.092E-01	9.565E-03	3.1	3.109E-01	9.306E-03	3.0
λ_5	1.224E+00	1.092E-01	8.9	1.244E+00	1.006E-01	8.1
λ_6	3.294E+00	2.696E-01	8.2	3.353E+00	2.609E-01	7.8
λ_{eff}	8.126E-02	3.004E-03	3.7	8.210E-02	3.184E-03	3.9

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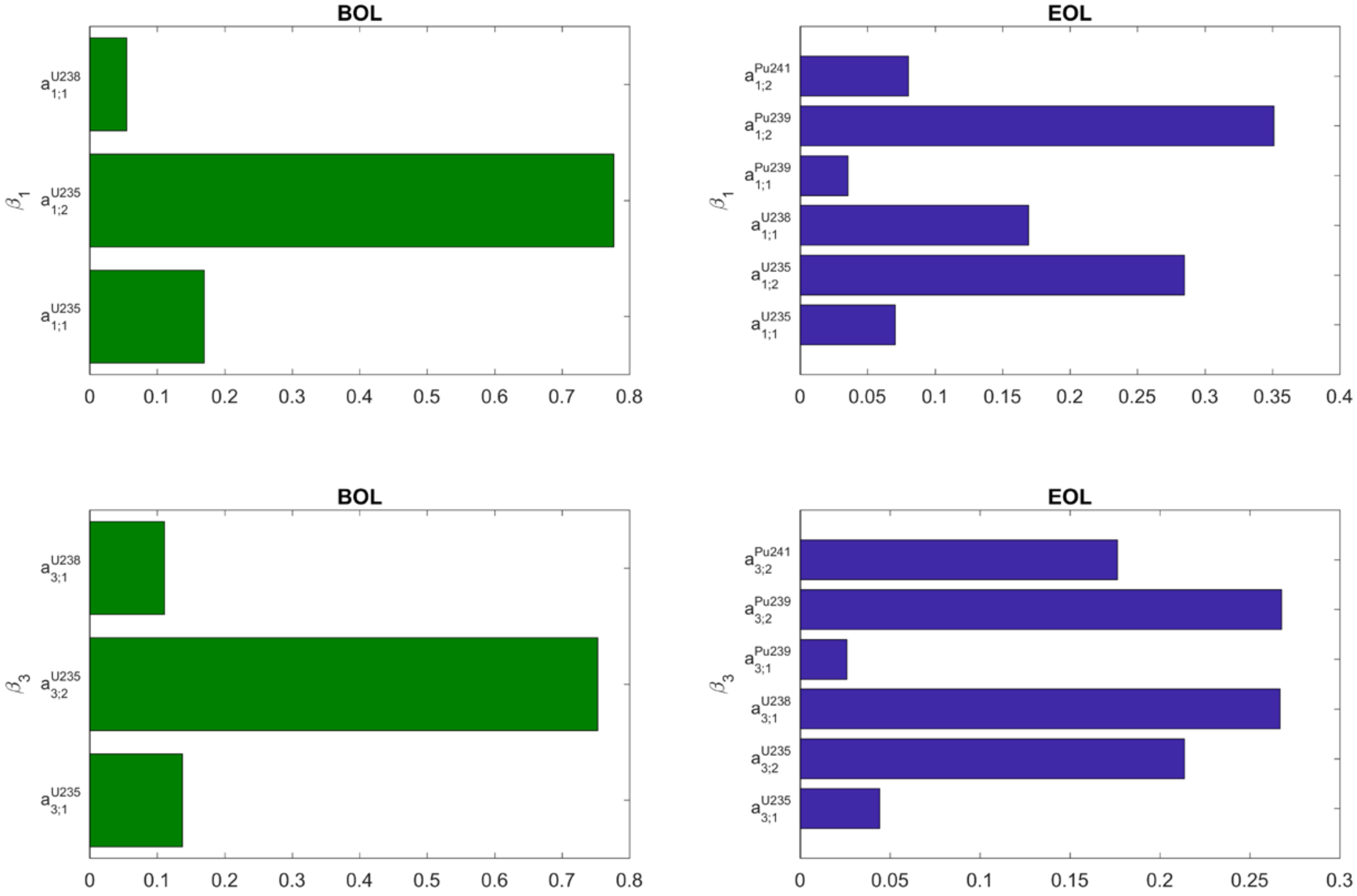
Beta Sensitivities



$X^{Isotope}_{i,g}$

Where:

$X = a, \lambda, Y$ (Parameter)

Isotope: U235, U238, etc.

$i = 1, 2, .., 6$ (Precursor group)

$g = 1, 2$ (Energy group)

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Input/output Relationship

- General input/output relationship

$$\vec{y} = f(\vec{x}) = f(x_1, x_2, ..., x_d) \qquad p(\vec{x}) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp[\tfrac{1}{2}(\vec{x}-\mu)^T \Sigma^{-1}(\vec{x}-\mu)]$$

- $f(x)$: could be a simulation code you use in your lab
- $\vec{x}$: a set of input parameters you provided to your code (e.g. density, thermal conductivity, etc.)
- $\vec{y}$: response calculated by the code (e.g. temperature, pressure, neutron flux, delayed neutron fraction)
- For demonstration:
  - Assume BOL (U-235, U-238).
  - Assume no correlation between parameters.

$$\vec{x}^{U235} = a_{1,1}^{U235}, ..., a_{6,1}^{U235}, a_{1,2}^{U235}, ..., a_{6,2}^{U235}, \lambda_{1,1}^{U235}, ..., \lambda_{6,1}^{U235}, \lambda_{1,2}^{U235}, ..., \lambda_{6,2}, Y_{,1}^{235}, Y_{,2}^{235} \quad (d=26)$$

$$\vec{x}^{U238} = a_{1,1}^{U238}, ..., a_{6,1}^{U238}, \lambda_{1,1}^{U235}, ..., \lambda_{6,1}^{U235}, Y_{,1}^{235} (d=13)$$

$$\vec{y} = \beta_1, \beta_2, ..., \beta_6, \beta_{eff}, \lambda_1, \lambda_2, ..., \lambda_6, \lambda_{eff} (d=14)$$

Reduced Order Modeling

Multiple Linear Regression (MLR) and Gaussian Process (GP)

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_{p-1} x_{i(p-1)} + \epsilon_i, \qquad i = 1, 2, \ldots, n$$

$$\epsilon_i \sim N(0, \sigma^2)$$

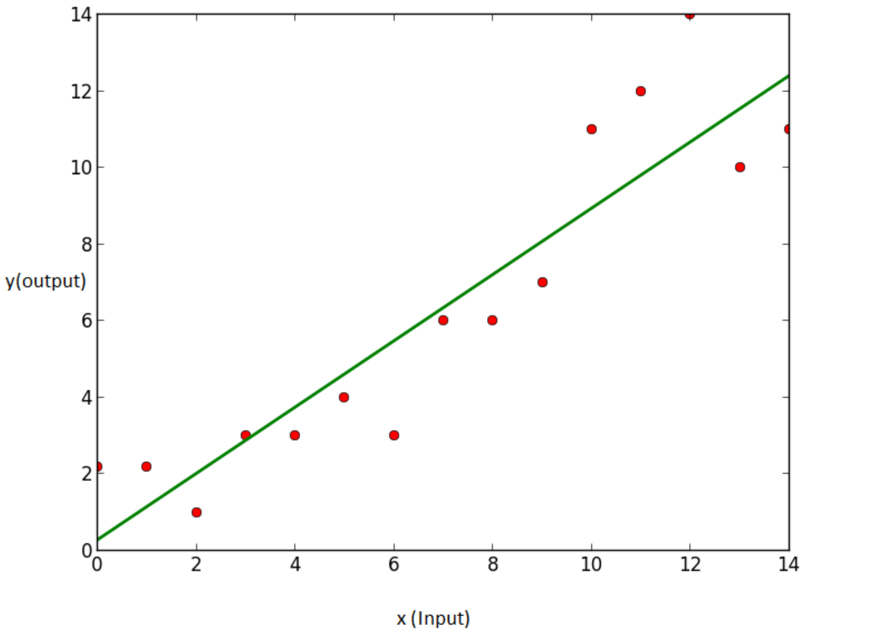
$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1(p-1)} \\ 1 & x_{21} & x_{22} & \cdots & x_{2(p-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{n(p-1)} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{p-1} \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

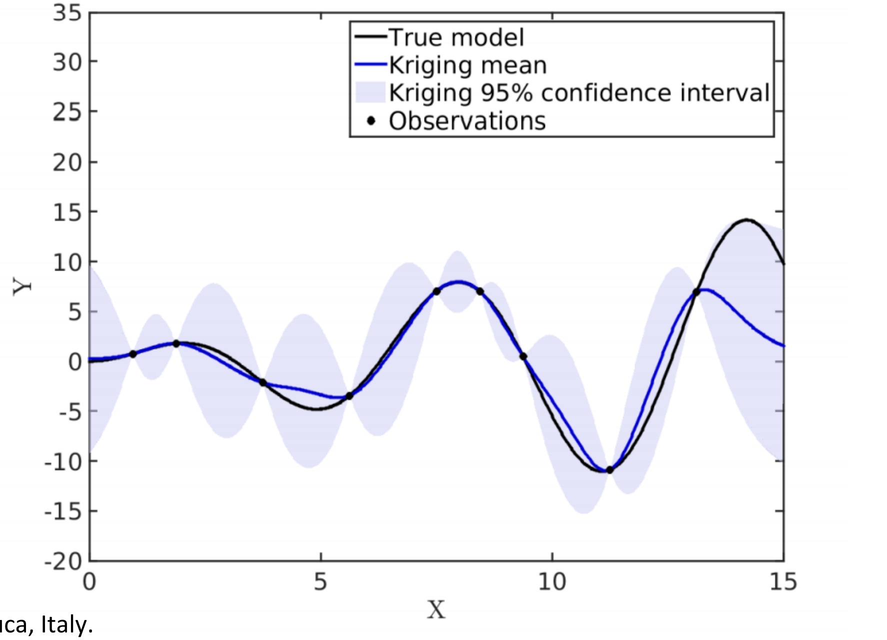
$$Y = X\beta + \epsilon$$

$$\vec{y} = [y_1, y_2, \ldots, y_n]^T$$

$$\mathbf{X} = [\vec{x}^1, \vec{x}^2, \ldots, \vec{x}^n]^T$$

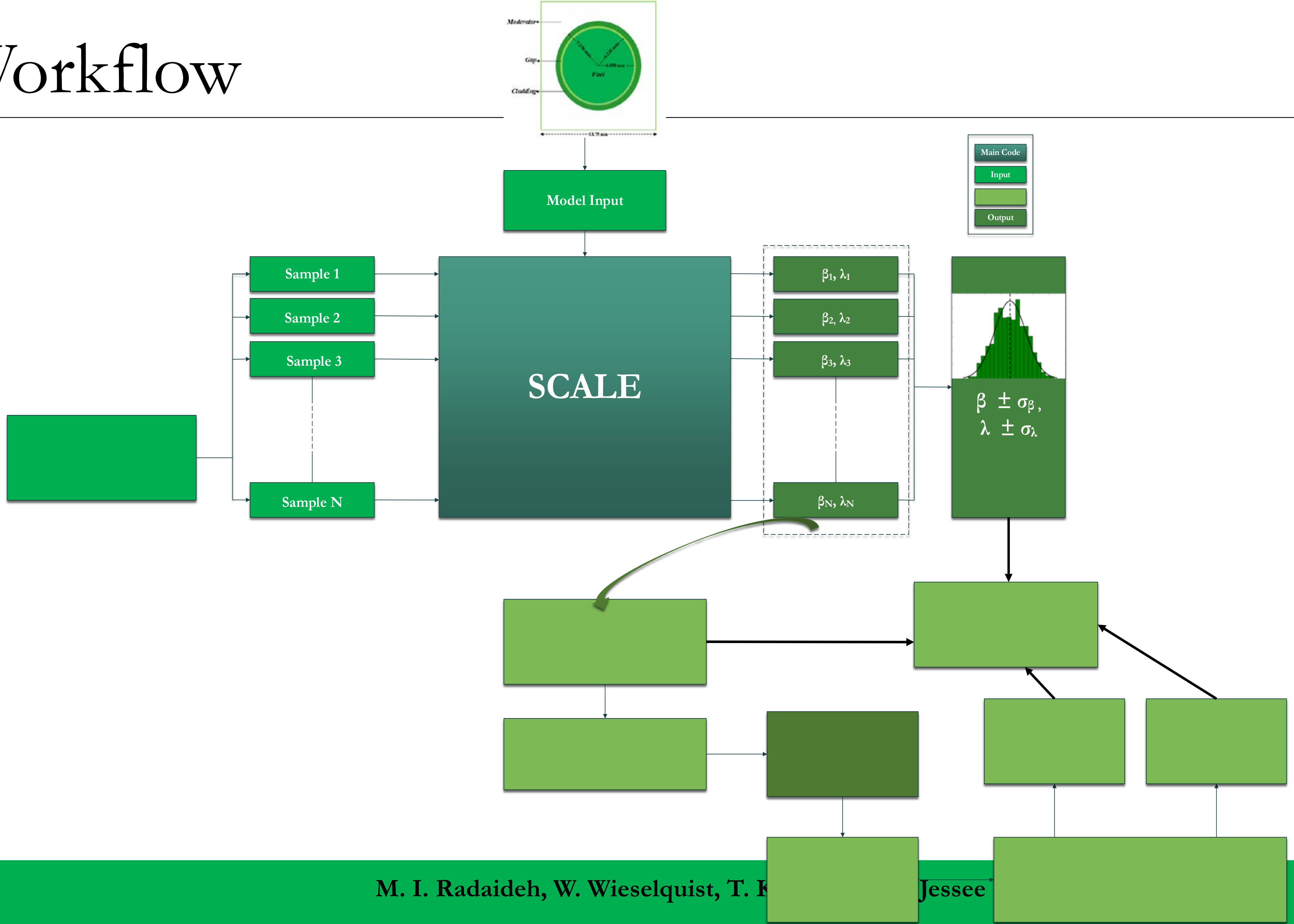
$$y(\vec{x}) = \sum_{i=0}^{k} \beta_i \phi_i(\vec{x}) + z(\vec{x})$$





[1] M.I. Radaideh, W. Wieslequist, T. Kozlowski. Sensitivity and Uncertainty Analysis of Delayed Neutron Data in LWRs, BEPU2018, May 13-19, Luuca, Italy.

Workflow



Moderator
Gap
Cladding
Fuel
Model Input
Main Code
Input
Output
Sample 1
Sample 2
Sample 3
Sample N
SCALE
β_1, λ_1
β_2, λ_2
β_3, λ_3
β_N, λ_N
$\beta \pm \sigma_\beta,$
$\lambda \pm \sigma_\lambda$

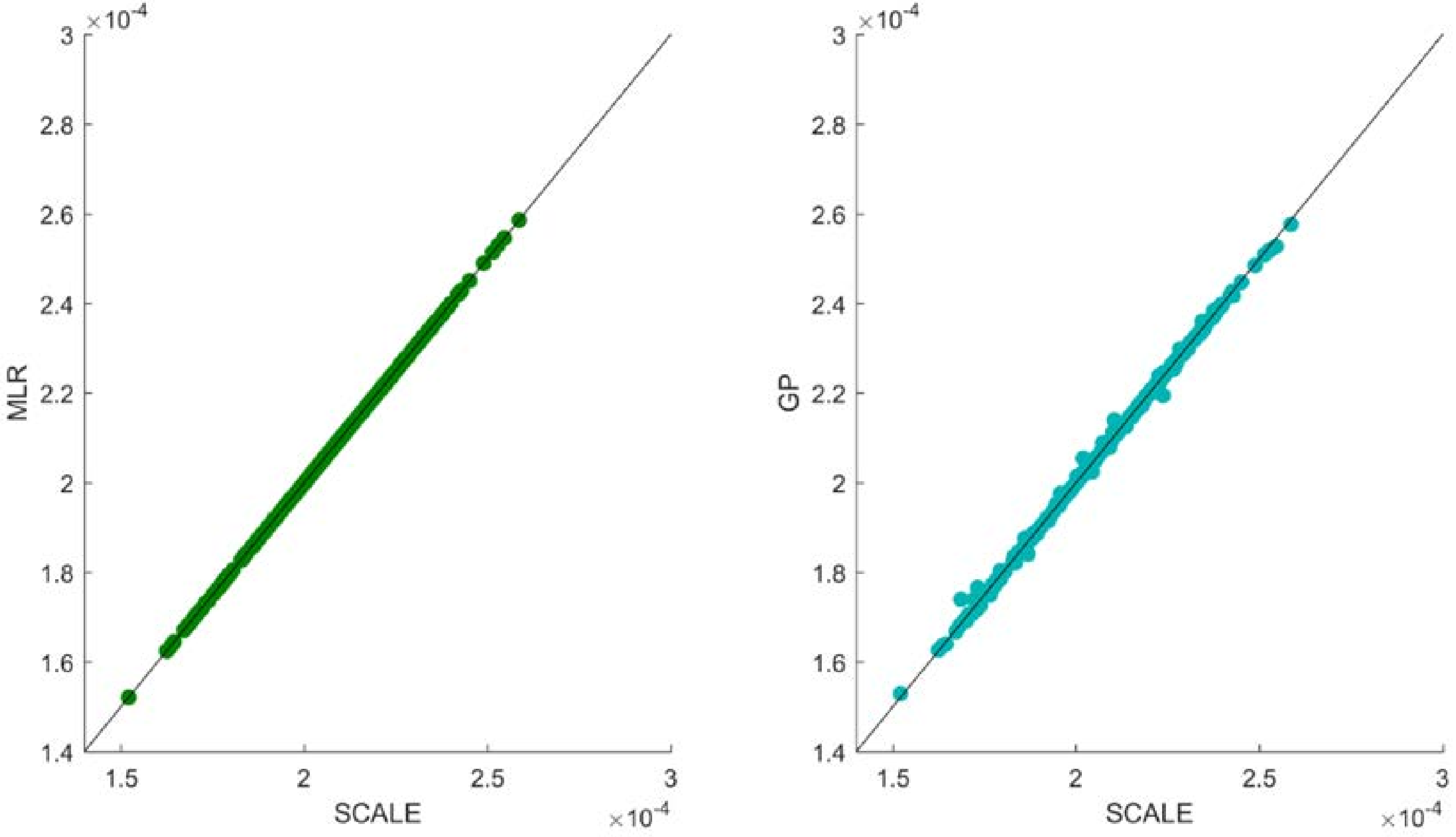
β_1 ROM

$$Q_2(Y,\hat{Y}) = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} \quad MSE = \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{n} \quad Corr(Y,\hat{Y}) = \frac{Cov(Y,\hat{Y})}{\sigma_Y \sigma_{\hat{Y}}}$$

- The data points that are shown are based on the validation set not training set to avoid overfitting.
- Advantage of linearity between DND and kinetic parameters.

Method	Q_2	MSE	Corr
MLR	0.998	8.42E-13	0.999
GP	0.996	1.35E-12	0.998

Multiple Linear Regression (MLR) and Gaussian Process (GP)



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ROM-based UQ

FOM: Full order model

Uncertainty propagated here is due to **DND only**. XS source was turned off.

β_1

Parameter	SCALE	FOM-MLR	ROM-MLR	ROM-GP
μ	2.0822E-04	2.0840E-04	2.0838E-04	2.0858E-04
σ	1.9196E-05	1.9076E-05	1.9143E-05	1.9162E-05
$\frac{\sigma}{\mu}\%$	9.22	9.15	9.19	9.20

λ_{eff}

Parameter	SCALE	FOM-MLR	ROM-MLR	ROM-GP
μ	8.3545E-02	8.3550E-02	8.3572E-02	8.3656E-02
σ	2.4675E-03	2.4319E-03	2.4045E-03	2.4069E-03
$\frac{\sigma}{\mu}\%$	2.95	2.91	2.88	2.88

Computational time based on 500 samples

SCALE	FOM-MLR	ROM-MLR	ROM-GP
41.7 hr	9.0E-03 s	4.0E-03 s	1.7 s

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Sobol Indices (Analysis of Response Variance)

$$S_i = \frac{D_i}{D} \qquad T_i = \frac{D_i^T}{D}$$

D : total response variance.
D_i: response variance from parameter x_i alone.
D_i^T: response variance from paramter x_i and its interactions with other parameters.

- S_i (First order index): describes the contribution to the output variance of the main effect of X_i, therefore it measures the effect of varying X_i alone.
- T_i (Total index): describes the contribution to the output variance of X_i, including all variances caused by its interactions, of any order, with any other input parameters.

$$\sum_{1\leq i\leq d} S_i + \sum_{1\leq i<j\leq d} S_{ij} + \sum_{1\leq i<j<k\leq d} S_{ijk} + \ldots = 1$$

Sobol Indices (Analysis of Response Variance)

$$S_i = \frac{D_i}{D} \qquad T_i = \frac{D_i^T}{D}$$

$$f_0 = \int_{D_X} f(\vec{x})p(\vec{x})d\vec{x}$$

$$D = \int_{D_X} f^2(\vec{x})p(\vec{x})d\vec{x} - f_0^2$$

$$D_i = \int_{D_X} f(\vec{x})p(\vec{x})f(x_i, \vec{x}'_{\sim i})p(\vec{x}'_{\sim i})dx$$

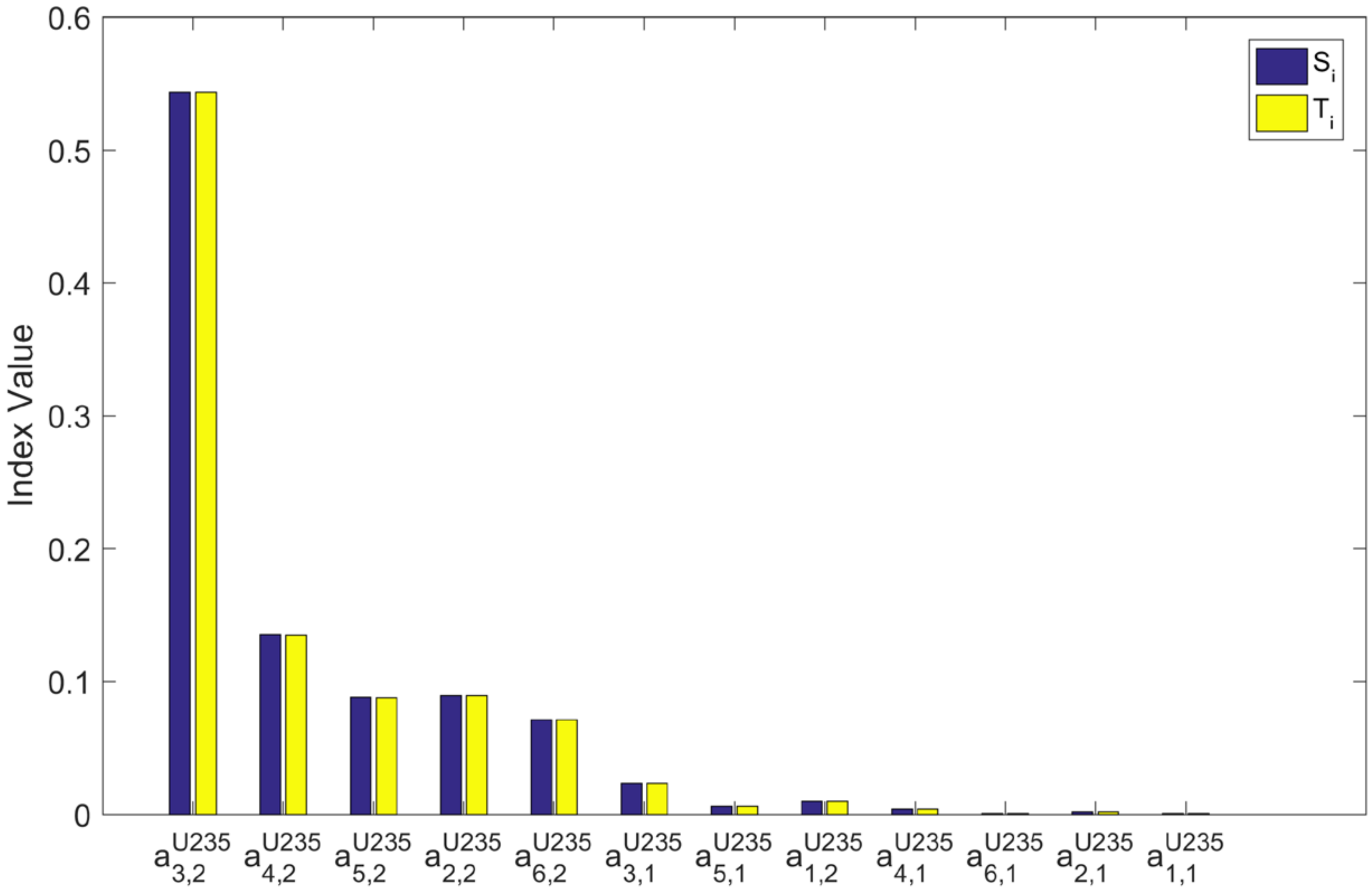
The notation $\sim i$ means all input paramters except i

$\vec{x}_{\sim i} = (x_1, ..., x_{i-1}, x_{i+1}, ..., x_d)$

- Analytical solution to the Sobol indices is not always found, Monte Carlo integration can be used

$\hat{f}_0 = \frac{1}{N}\sum_{i=1}^{N} f(x^{(i)})$ where $x^{(i)}$ are iid samples from $p(\vec{x})$

β_{eff} Sobol Indices (BOL)



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Where:

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Summary

- A data-driven approach sampling-based approach for UQ of kinetic parameters was developed.
- The new approach includes the uncertainty in the measured precursor group parameters in kinetic parameters calculations.
- Uncertainty provided here is expected to be higher than the usual approach of β_{eff} calculations (k-ratio) since additional input paramtetrs are considered.
- The framework is flexible and can be used in various applications such as sensitivity analysis, reduced order modeling, data assimilation, and variance decomposition.

Our Publications (for more info)

- The kinetics UQ framework was firstly introduced sat **PHYSOR-2018 (Mexico)**.
- The PHYSOR paper is selected later for publication at its special issue (will appear in **Annals of Nuclear Energy** by the end of this year).
- Improving the flexibility of the framework for sensitivity, ROM, and ROM-based UQ was introduced at **BEPU-2018 (Italy)**.
- A rigorous variance-based sensitivity analysis of the DND using Sobol decomposition methods will be introduced at **PHYTRA4 (Morocco).**
- A journal article about the framework development with a comprehensive look on kinetic parameters' sensitivity and uncertainty will be submitted to **Nuclear Engineering and Design** soon.

Thank You!

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- R. Waldo, R. Karam, R. Meyer, Delayed neutron yields: Time dependent measurements and a predictive model, Physical Review C 23 (3) (1981) 1113.
- D. J. Loaiza, G. Brunson, R. Sanchez, K. Butterfield, Measurements of Absolute Delayed Neutron Yield and Group Constants in the Fast Fission of ^{235}U and ^{237}Np, Nuclear science and engineering 128 (3) (1998) 270–277.
- G. R. Keepin, T. Wimett, R. Zeigler, Delayed neutrons from fissionable isotopes of uranium, plutonium, and thorium, Physical review 107 (4) (1957) 1044.
- H. H. Saleh, T. A. Parish, S. Raman, N. Shinohara, Measurements of delayed neutron decay constants and fission yields from ^{235}U, ^{237}Np, ^{241}Am, and ^{243}Am, Nuclear science and engineering 125 (1) (1997) 51–60.

- D. J. Loaiza, G. Brunson, R. Sanchez, K. Butterfield, Measurements of Absolute Delayed Neutron Yield and Group Constants in the Fast Fission of ^{235}U and ^{237}Np, Nuclear science and engineering 128 (3) (1998) 270–277.

- M. I. Radaideh, W. Wieselquist, T. Kozlowski, Sampling-Based Uncertainty Quantitation of the Six-group Kinetic Parameters, Proc. Physics of Reactors (PHYSOR-2018), Cancun, Mexico, April 22-26, 2018 .
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