A New SCALE Capability for Uncertainty Quantification of Kinetic Parameters

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Presented by:

Majdi I. Radaideh (PhD Candidate at UIUC)
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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 ($\beta_{eff}, \beta_i, \lambda_i, \lambda_{eff}$) averaged over all isotopes are needed along with their uncertainty.

• At the end, you provide a single value of each kinetic parameter (e.g. $\beta_{eff}$) which represents the average of all delayed neutron emitters.

• The sources of uncertainty:
  1. Fundamental Nuclear Data: XS (e.g. $\nu, \Sigma_f, \chi$)
  2. Fundamental Delayed Neutron Data: DND (e.g. $a_{j,i}, \lambda_{j,i}$)

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

\[
\frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t), \quad (i = 1, ..., N)
\]

Response of Interest (Homogenized Kinetic Parameters):

\[
\beta_{j,i} = a_{j,i} Y_j
\]

\[
\beta_i = \sum_j \beta_{j,i} \sum_m \sum_g \bar{\nu} \Sigma_f^{j,m,g} \varphi_{m,g} V_m \sum_{g_r} \chi_{d,i}^{g_r} \varphi_{g_r}^{*}
\]

\[
\frac{\sum_j \sum_m \sum_g \bar{\nu} \Sigma_f^{j,m,g} \varphi_{m,g} V_m \sum_{g_r} \chi^{g_r} \varphi_{g_r}^{*}}{\sum_j \sum_m \sum_g \bar{\nu} \Sigma_f^{j,m,g} \varphi_{m,g} V_m}
\]

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

\[
\lambda_{eff} = \sum_{i=1}^{N} \frac{\beta_i}{\lambda_i}
\]

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• Background

• **The Framework Description**

• Preliminary Analysis

• Applications
  • Sensitivity Analysis
  • Reduced Order Modeling
  • ROM-based UQ
  • Variance Decomposition by Sobol indices

• Summary
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 $X_{Isotope}^{I,g}$  

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

- Examples:  
$a_{U^{235}}^{1,2}$  
$\lambda_{U^{238}}^{2,1}$

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

<table>
<thead>
<tr>
<th>Isotope</th>
<th>No.</th>
<th>$a_{i,j}$ (F)</th>
<th>$\lambda_{i,j}$ (F)</th>
<th>$a_{i,j}$ (T)</th>
<th>$\lambda_{i,j}$ (T)</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-233</td>
<td>1</td>
<td>0.086 ± 0.004</td>
<td>0.0126 ± 0.0006</td>
<td>0.086 ± 0.003</td>
<td>0.0126 ± 0.0001</td>
<td>F: Tuttle (1975)</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.274 ± 0.007</td>
<td>0.0334 ± 0.0021</td>
<td>0.299 ± 0.004</td>
<td>0.0337 ± 0.0006</td>
<td>T: Keepin et al. (1957)</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.227 ± 0.052</td>
<td>0.1310 ± 0.0370</td>
<td>0.252 ± 0.040</td>
<td>0.1386 ± 0.0058</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>0.317 ± 0.018</td>
<td>0.3020 ± 0.0360</td>
<td>0.278 ± 0.020</td>
<td>0.3254 ± 0.0306</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>0.073 ± 0.021</td>
<td>1.2700 ± 0.3900</td>
<td>0.051 ± 0.024</td>
<td>1.1271 ± 0.4435</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>0.023 ± 0.010</td>
<td>3.1300 ± 1.0000</td>
<td>0.034 ± 0.014</td>
<td>2.5023 ± 0.4246</td>
<td></td>
</tr>
</tbody>
</table>

| Pu-239  | 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 ± 0.000 | 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 | 0.3210 ± 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    |        |

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

## 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.

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

*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 not available in either Tuttle (1975) or Keepin et al. (1957), a different source is used for the group parameters and absolute yield.

• If there is no experimental data available for the group parameters of a specific isotope, a computational-based data source was selected from Wilson and England (2002). The computational data has no uncertainty and hence had no effect on the UQ results.

• If there is no experimental data available for nubar (delayed) of a specific isotope in delayed neutron experiments, the value and its uncertainty were taken from SCALE data and covariance libraries which are based on ENDF-B/VII.1.

• All nubar and its uncertainty for all isotopes was taken from SCALE data and covariance libraries based on ENDF-B/VII.1. Exceptions to the previous points were minimal, and they are mentioned in the appropriate place in the text.
The Framework Features

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 ($\beta_i$)

- Note: the spread is caused by uncertainties in DND and XS
  $\beta_{\text{eff}}$ uncertainty $\sim$ 7-9%

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

Group-Wise Lambda Uncertainty ($\lambda_i$)

- 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 $\pm 1\sigma$ 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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>TRITON</th>
<th></th>
<th>Polaris</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Std</td>
<td>Relative(%)</td>
<td>Mean</td>
</tr>
<tr>
<td>$\beta_1$</td>
<td>2.112E-04</td>
<td>1.755E-05</td>
<td>8.3</td>
<td>2.124E-04</td>
</tr>
<tr>
<td>$\beta_2$</td>
<td>1.412E-03</td>
<td>8.752E-05</td>
<td>6.2</td>
<td>1.415E-03</td>
</tr>
<tr>
<td>$\beta_3$</td>
<td>1.291E-03</td>
<td>1.432E-04</td>
<td>11.1</td>
<td>1.299E-03</td>
</tr>
<tr>
<td>$\beta_4$</td>
<td>2.689E-03</td>
<td>1.992E-04</td>
<td>7.4</td>
<td>2.725E-03</td>
</tr>
<tr>
<td>$\beta_5$</td>
<td>8.882E-04</td>
<td>1.131E-04</td>
<td>12.7</td>
<td>9.197E-04</td>
</tr>
<tr>
<td>$\beta_6$</td>
<td>2.988E-04</td>
<td>5.305E-05</td>
<td>17.8</td>
<td>3.020E-04</td>
</tr>
<tr>
<td>$\beta_{eff}$</td>
<td>6.790E-03</td>
<td>5.064E-04</td>
<td>7.5</td>
<td>6.873E-03</td>
</tr>
<tr>
<td>$\lambda_1$</td>
<td>1.249E-02</td>
<td>2.411E-04</td>
<td>1.9</td>
<td>1.252E-02</td>
</tr>
<tr>
<td>$\lambda_2$</td>
<td>3.081E-02</td>
<td>7.982E-04</td>
<td>2.6</td>
<td>3.089E-02</td>
</tr>
<tr>
<td>$\lambda_3$</td>
<td>1.148E-01</td>
<td>3.572E-03</td>
<td>3.1</td>
<td>1.155E-01</td>
</tr>
<tr>
<td>$\lambda_4$</td>
<td>3.092E-01</td>
<td>9.565E-03</td>
<td>3.1</td>
<td>3.109E-01</td>
</tr>
<tr>
<td>$\lambda_5$</td>
<td>1.224E+00</td>
<td>1.092E-01</td>
<td>8.9</td>
<td>1.244E+00</td>
</tr>
<tr>
<td>$\lambda_6$</td>
<td>3.294E+00</td>
<td>2.696E-01</td>
<td>8.2</td>
<td>3.353E+00</td>
</tr>
<tr>
<td>$\lambda_{eff}$</td>
<td>8.126E-02</td>
<td>3.004E-03</td>
<td>3.7</td>
<td>8.210E-02</td>
</tr>
</tbody>
</table>
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Beta Sensitivities

\[ X_{i,g}^{Isotope} \]

Where:
\[ X = a, \lambda, Y \text{ (Parameter)} \]
Isotope: U235, U238, etc.
\[ i = 1, 2, ..., 6 \text{ (Precursor group)} \]
\[ g = 1, 2 \text{ (Energy group)} \]
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Input/output Relationship

• General input/output relationship

\[ \vec{y} = f(\vec{x}) = f(x_1, x_2, \ldots, x_d) \]

\[ p(\vec{x}) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left[\frac{1}{2}(\vec{x} - \mu)^T \Sigma^{-1} (\vec{x} - \mu)\right] \]

• \( f(x) \): 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.

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

\[ \vec{x}^{U238} = a_{1,1}^{U238}, a_{6,1}^{U238}, \lambda_{1,1}^{U238}, \ldots, \lambda_{6,1}^{U238}, Y_{1,235}^{235} \quad (d = 13) \]

\[ \vec{y} = \beta_1, \beta_2, \ldots, \beta_6, \beta_{eff}, \lambda_1, \lambda_2, \ldots, \lambda_6, \lambda_{eff} \quad (d = 14) \]
Reduced Order Modeling

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

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

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

\[ \epsilon_i \sim N(0, \sigma^2) \]

\[ Y = X \beta + \epsilon \]

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

\[ X = [\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n]^T \]

\[ y(\vec{x}) = \sum_{i=0}^{K} \beta_i \phi_i(\vec{x}) + z(\vec{x}) \]

Workflow

\[ \beta_1 \text{ ROM} \]

\[ Q_2(Y, \hat{Y}) = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} \]

\[ \text{MSE} = \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{n} \]

\[ \text{Corr}(Y, \hat{Y}) = \frac{\text{Cov}(Y, \hat{Y})}{\sigma_Y \sigma_{\hat{Y}}} \]

- 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.

<table>
<thead>
<tr>
<th>Method</th>
<th>( Q_2 )</th>
<th>MSE</th>
<th>Corr</th>
</tr>
</thead>
<tbody>
<tr>
<td>MLR</td>
<td>0.998</td>
<td>8.42E-13</td>
<td>0.999</td>
</tr>
<tr>
<td>GP</td>
<td>0.996</td>
<td>1.35E-12</td>
<td>0.998</td>
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</table>

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

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ROM-based UQ

FOM: Full order model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SCALE</th>
<th>FOM-MLR</th>
<th>ROM-MLR</th>
<th>ROM-GP</th>
</tr>
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<tbody>
<tr>
<td>$\mu$</td>
<td>2.0822E-04</td>
<td>2.0840E-04</td>
<td>2.0838E-04</td>
<td>2.0858E-04</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>1.9196E-05</td>
<td>1.9076E-05</td>
<td>1.9143E-05</td>
<td>1.9162E-05</td>
</tr>
<tr>
<td>$\sigma_\mu$ %</td>
<td>9.22</td>
<td>9.15</td>
<td>9.19</td>
<td>9.20</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>SCALE</th>
<th>FOM-MLR</th>
<th>ROM-MLR</th>
<th>ROM-GP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$</td>
<td>8.3545E-02</td>
<td>8.3550E-02</td>
<td>8.3572E-02</td>
<td>8.3656E-02</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>2.4675E-03</td>
<td>2.4319E-03</td>
<td>2.4045E-03</td>
<td>2.4069E-03</td>
</tr>
<tr>
<td>$\sigma_\mu$ %</td>
<td>2.95</td>
<td>2.91</td>
<td>2.88</td>
<td>2.88</td>
</tr>
</tbody>
</table>

Computational time based on 500 samples

<table>
<thead>
<tr>
<th></th>
<th>SCALE</th>
<th>FOM-MLR</th>
<th>ROM-MLR</th>
<th>ROM-GP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>41.7 hr</td>
<td>9.0E-03 s</td>
<td>4.0E-03 s</td>
<td>1.7 s</td>
</tr>
</tbody>
</table>

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

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Sobol Indices (Analysis of Response Variance)

\[ S_i = \frac{D_i}{D} \quad T_i = \frac{D_i^T}{D} \]

- **\( S_i \) (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)

\[ S_i = \frac{D_i}{D}, \quad T_i = \frac{D_i^T}{D} \]

\[ f_0 = \int_{D_X} f(\bar{x})p(\bar{x})d\bar{x} \]

\[ D = \int_{D_X} f^2(\bar{x})p(\bar{x})d\bar{x} - f_0^2 \]

\[ D_i = \int_{D_X} f(\bar{x})p(\bar{x})f(x_i, \bar{x}_{\sim i})p(\bar{x}_{\sim i})dx \quad \text{The notation } \sim i \text{ means all input parameters except } i \]

\[ \bar{x}_{\sim i} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d) \]

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

\[ \hat{f}_0 = \frac{1}{N} \sum_{i=1}^{N} f(x^{(i)}) \text{ where } x^{(i)} \text{ are iid samples from } p(\bar{x}) \]
**$\beta_{eff}$ Sobol Indices (BOL)**

Where:
- $X = a, \lambda, Y$ (Parameter)
- Isotope: U235, U238, etc.
- $i = 1, 2, \ldots, 6$ (Precursor group)
- $g = 1, 2$ (Energy group)
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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 $\beta_{eff}$ calculations (k-ratio) since additional input parameters 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 at 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!