METHODS AND APPROACHES DEVELOPMENT AT ORNL FOR PROVIDING FEEDBACK FROM INTEGRAL BENCHMARK EXPERIMENTS FOR IMPROVEMENT OF NUCLEAR DATA FILES

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<td>SAMINT: A Code for Nuclear Data Adjustment with SAMMY Based on Integral Experiments</td>
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<td>2</td>
<td>INSURE: INverse Sensitivity/UnceRTainty Estimator</td>
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SAMINT: A Code for Nuclear Data Adjustment with SAMMY Based on Integral Experiments

- Allow coupling of differential and integral data evaluation in a continuous-energy framework
- Update the resonance parameter evaluation directly based on integral benchmark experiments
Integral Experiments to Aid Nuclear Data Evaluation

• SAMINT can be used to extract information from integral benchmarks to aid the nuclear data evaluation process.

• Near the end of the evaluation based on differential experimental data, integral data can be used to:
  • Resolve remaining ambiguity between differential data sets
  • Guide the evaluator to troublesome energy regions
  • Inform the evaluator of the most important nuclear data parameters to integral benchmark calculations
  • Improve the nuclear data covariance matrix evaluation
SAMINT Proper Uses

- **SAMINT is not intended** to bias the nuclear data towards fitting a certain set of integral experiments.
- SAMINT should be used to **supplement** evaluation of differential experimental data.
- Using the GLLS methodology ensures that the updated nuclear data parameters respect the original fit of the differential data.
Using SAMINT with SAMMY

Differential Experimental Data

\[ \frac{d\sigma(E)}{dP} \]

\[ \frac{dk}{dP} \]

\[ \frac{dk}{d\sigma(E)} \]

Integral Experimental Data

P stands for all resonance parameters: \( E_\lambda, \Gamma_\gamma, \Gamma_n, \Gamma_f \), etc.
SAMINT Capabilities for Initial Release from RSICCC

• Current Capabilities
  – Adjusting resolved resonance parameters and associated covariance
  – Adjusting number of prompt neutrons per fission
  – Calculating continuous energy cross sections and eta values (reactor physics) to satisfy integral benchmarks
  – Works with both CE TSUNAMI and MCNP-6 k-eigenvalue sensitivities
  – Iteration for non-linearity
SAMINT Release Through RSICCC

- SAMINT will be distributed with the SAMMY code from RSICCC! [https://rsicc.ornl.gov/](https://rsicc.ornl.gov/)
- Optional compile-time inclusion
- LAPACK/BLAS for all linear algebra operations
- Mac, Linux, Windows
- Version control
- Automated test cases

<table>
<thead>
<tr>
<th>Case Name</th>
<th>SAMINT Capability</th>
<th>Sensitivity Code</th>
<th>Notes</th>
</tr>
</thead>
</table>
| tr181     | - Resonance Parameter updating  
- Eta updating with correlations  
- Eta updating without correlations  
- Integral experiment covariance matrix | CE TSUNAMI-3D | Independently confirmed by MATLAB calculations |
| tr182     | - $^{56}$Fe case  
- Fitting resonance parameters with inelastic channel open | MCNP6 | Complication comes from appearance of zero cross-sections due to threshold reactions |
| tr183     | - $^{239}$Pu case  
- Fitting resonance parameter and nu-bar simultaneously  
- Independent eta updating | MCNP6 | |

Sample Calculations

• As a demonstration calculation, SAMINT was used to adjust the resolved resonance region evaluation of $^{56}$Fe.

• Four integral experiments from the ICSBEP were selected.

• Energy region of evaluation: 1e-5 eV to 2 MeV.

• 1190 resonance parameters varied:
  - $\Gamma_\gamma$: 450 keV – 2MeV
  - $\Gamma_{(n,n')1}$ and $\Gamma_{(n,n')2}$: 846 keV – 2MeV
Inelastic cross section of $^{56}\text{Fe}$ before ($\chi^2 = 73.3382$) and after ($\chi^2 = 73.6877$) the adjustment based on integral experimental data plotted on top of differential experimental data of Plompen, presented with one standard deviation error bars.
Inelastic cross section of $^{56}$Fe before ($\chi^2 = 23.6023$) and after ($\chi^2 = 22.9036$) the adjustment based on integral experimental data plotted on top of differential experimental data of Perey, presented with one standard deviation error bars.
**56Fe Results**

- **C/E:** Computed Value
  Experimentally Measured Value

<table>
<thead>
<tr>
<th>Integral Experiment Name</th>
<th>Before Adjustment</th>
<th>After Adjustment</th>
</tr>
</thead>
<tbody>
<tr>
<td>HMF013</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HMF021</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PMF025</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PMF032</td>
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Expanded Capabilities

First Update Release (Spring)

• Cross-Isotope correlation matrices
  – Determine the posterior correlation matrix created by adjusting several isotopes simultaneously

• Use of Angular Distribution Sensitivity with MCNP6 for adjusting resonance parameters

• Immediate application: $^{63}\text{Cu}$ and $^{65}\text{Cu}$

In FY2016

• Extension to Unresolved Resonance Region

• Support of Generalized Sensitivity Capabilities of CE TSUNAMI-3D
Summary

• SAMINT should be used to **supplement** evaluation of differential experimental data.

• SAMINT will also improve the nuclear data covariance matrix evaluation.

• Plans to extend the SAMINT methodology to the unresolved resonance region and the high energy region.

• Support for this work was provided by the US DOE Nuclear Criticality Safety Program.
INSURE: INverse Sensitivity/UnceRtainty Estimator

• Determine target accuracies of nuclear data needed to model applications within prescribed tolerances

• Minimize the cost of acquiring improved data that would yield acceptable uncertainties of responses
Applications

Application Examples:

• Light Water Reactors
• Fast neutron reactors
• Spent Nuclear Fuel
  – Reprocessing
  – Transport
  – Disposal

Response Examples

– Neutron multiplication factor
– Cycle length
– Power distribution
– Reaction rate ratio
Inverse S/U: Definitions

• A nuclear application design specifies maximum allowed uncertainties on performance parameters (“responses”)
  – e.g. the multiplicity factor and its tolerance
    \[ R \pm \Delta R \]

• Neutron transport using existing cross section uncertainties often leads to an application response uncertainty greater than the maximum allowed, i.e.:
  \[ \sigma_0 \pm \Delta \sigma_0 \Rightarrow R_0 \pm \Delta R_0 \quad \text{where} \quad \Delta R_0 > \Delta R \]

• Inverse S/U: What set of improved data would lower the response uncertainty below the specified tolerance?
  – While minimizing the cost of data measurements
    \[ \sigma' \pm \Delta \sigma' \Rightarrow R' \pm \Delta R' \leq \Delta R \quad \text{for} \quad \min(\text{cost}[\Delta \sigma']) \]
Inverse S/U Math

• Given a desired responses ± tolerances: \( R \pm \Delta R \)
• And the existing data ± uncertainties: \( \sigma_0 \pm \Delta \sigma_0 \)
• Minimize the cost of acquiring improved data uncertainties that yield a response uncertainty within tolerance:

\[
\text{min}\{\text{Cost}[\Delta \sigma]\} \quad \text{such that} \quad S(\Delta \sigma)^2 S^T \leq (\Delta R)^2 \\
S = \left. \frac{\delta R(x)}{\delta \sigma} \right|_{\sigma = \sigma_0}
\]

• This is a constrained optimization problem:
  – MINCON: open source subroutine is used by MATLAB and DAKOTA
Including Integral Benchmark Experiments in IS/U

- Differential data uncertainties are limited by experimental methods
- Some data already at the present-day limits of experimental precision
- Uncertainties required by IS/U lower than these may be unrealistic

Table II. Uncertainties of the present-day state-of-the-art measurements for various cross sections

<table>
<thead>
<tr>
<th>Reaction</th>
<th>MT</th>
<th>Min. Rel. Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fission</td>
<td>18</td>
<td>0.7%</td>
</tr>
<tr>
<td>Capture</td>
<td>102</td>
<td>2%</td>
</tr>
<tr>
<td>Neutron yields</td>
<td>452</td>
<td>0.3%</td>
</tr>
<tr>
<td>Elastic scattering</td>
<td>2</td>
<td>2%</td>
</tr>
</tbody>
</table>

- IS/U results obtained with integral benchmark experiments afford larger differential data uncertainties, i.e.: lower cost of differential data
Including Integral Benchmark Experiments in IS/U

\[ \Delta \sigma \rightarrow \text{TSURFER} \rightarrow \Delta R \rightarrow \Delta R_{IBE} \rightarrow \Delta \sigma' \]

\[ \text{Integral Benchmark Experiment} \]

\[ \Delta R'_{IBE} \rightarrow \Delta R' \]

\[ \Delta \sigma \rightarrow \text{TSURFER} \rightarrow \Delta R \rightarrow \Delta R_{IBE} \rightarrow \Delta \sigma' \]
Example Calculations

• For PWR fuel array:
  • for extant data \( dk_{\text{eff}} = 0.0031 \)
  • we desire \( dk_{\text{eff}} = 0.0010, \text{var}(k_{\text{eff}})=10^{-6} \)

<table>
<thead>
<tr>
<th>TABLE I.  SUMMARY OF INVERSE S/U RESULTS</th>
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<tbody>
<tr>
<td>w/o Benchmark</td>
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<tr>
<td>Cost (arb.)</td>
</tr>
<tr>
<td>\text{var}(k_{\text{eff}})</td>
</tr>
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</table>

• An overall 6-fold decrease in data cost was achieved by including integral benchmarks in the Inverse S/U calculations.

• The integral benchmark experiment used in this work is water-moderated UO\(_2\) fuel rods in 2.032-cm square-pitched arrays (LEU-COMP-THERM-001). This experiment was chosen because of its similarity to the PWR fuel-rods.
Cost Function

• So far, the cost of a differential experiment has been assumed to be inversely proportional with the uncertainty in the differential data.

• A realistic cost function would account for:
  – duration of measurements
    • Needed to run the facility, pay the staff, etc.
    • Inversely proportional to the cross section
      – Smaller cross section requires longer run times
  – Cost of the target
    • manufactured or borrowed?
  – In collaboration with Klaus Guber we are devising more realistic cost functions.
Inverse S/U Results

Required relative uncertainties (benchmark vs. no benchmark) for neutron capture cross section (i.e. MT=102) for U-235 (left) and for U-238 (right). The plots show that inclusion of a benchmark affords less stringent uncertainties.
For U-235 neutron yield (MT=452) extant uncertainties (green) are already near (or smaller than) the ENDF guidance value of 0.3%. Here too, the IS/U with integral benchmark experiment (IBE) (red) require uncertainties that are not as small as those w/o IBEs (blue).
Summary

• A new application of the Inverse Sensitivity/Uncertainty to cost-optimized prioritization of nuclear data measurements

• Demonstrated the benefit of using integral benchmarks in the IS/U
  – Without integral benchmark experiments differential data uncertainties may be unachievable

• IS/U capability can be used for various nuclear fuel cycle applications
Outlook

• Formalism sufficiently general to minimize the TOTAL cost of data
  – Differential data and integral benchmark experiments simultaneously
  – Can be adapted to optimize systematic and statistical uncertainties simultaneously
  – It may be extended to optimize and design integral benchmark experiment

• Complexity reduction methods developed by Hany Abdel-Khalik are being applied to decrease the computational load for more complex responses
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