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

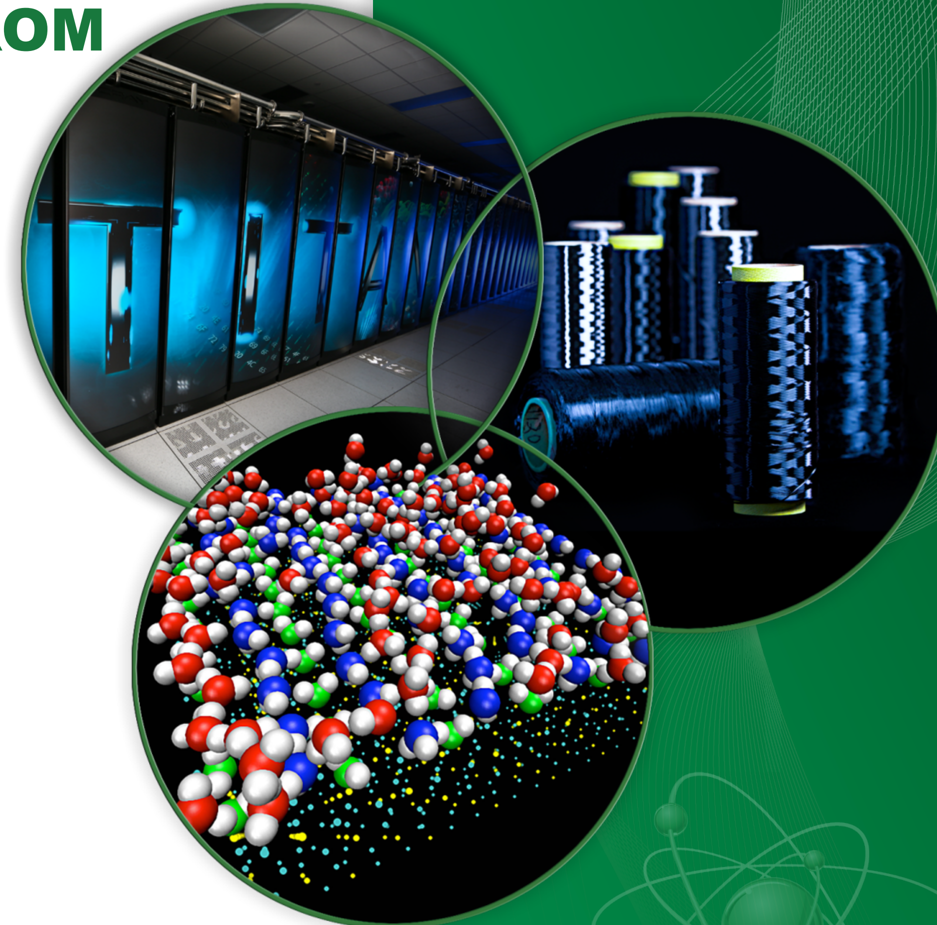

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Table of Content

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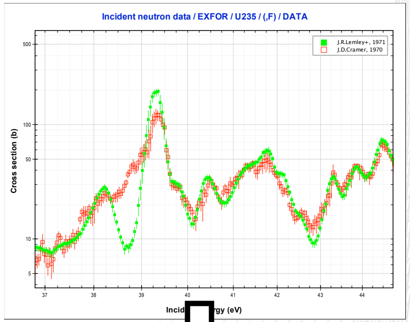
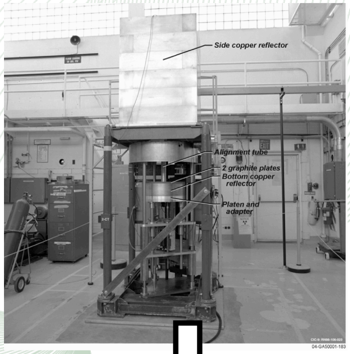
SAMINT: A Code for Nuclear Data Adjustment with SAMMY Based on Integral Experiments

- 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



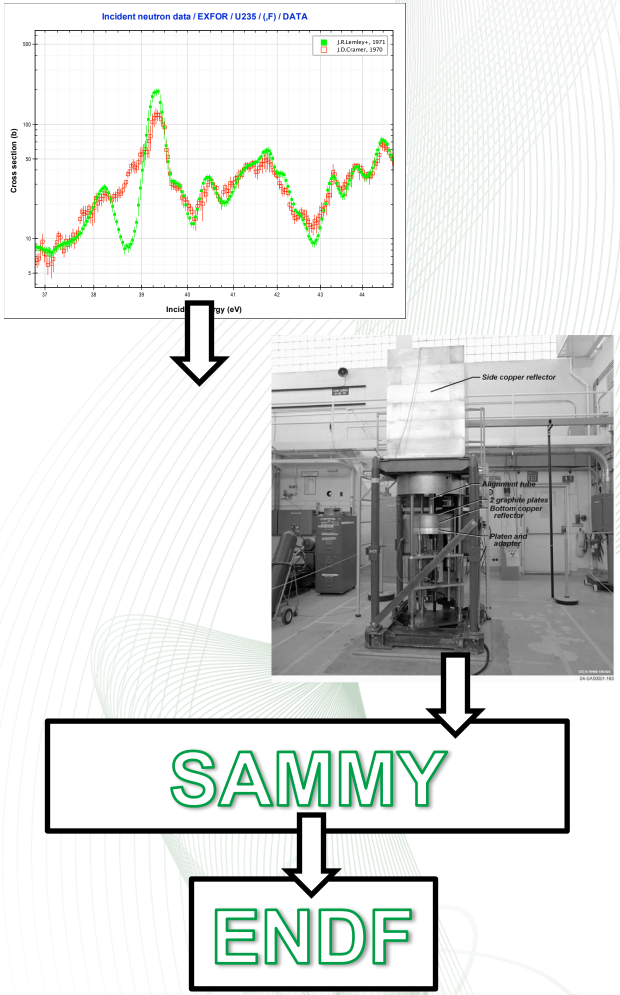


SAMMY

ENDF

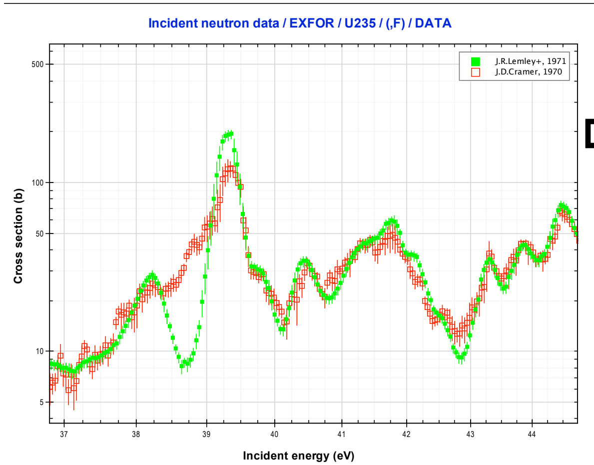
SAMINT
Proper Uses

- 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

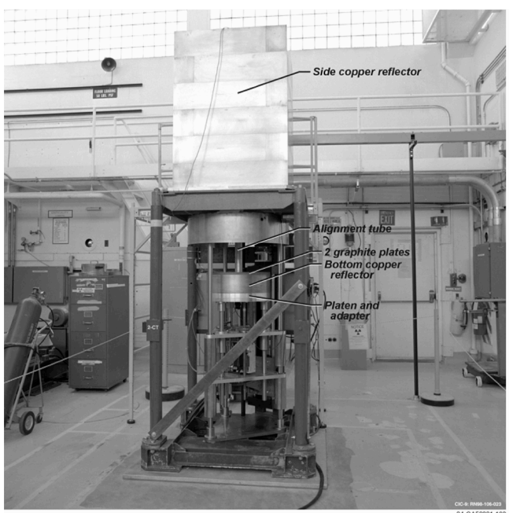


Using SAMINT with SAMMY

Differential Experimental Data



Integral Experimental Data

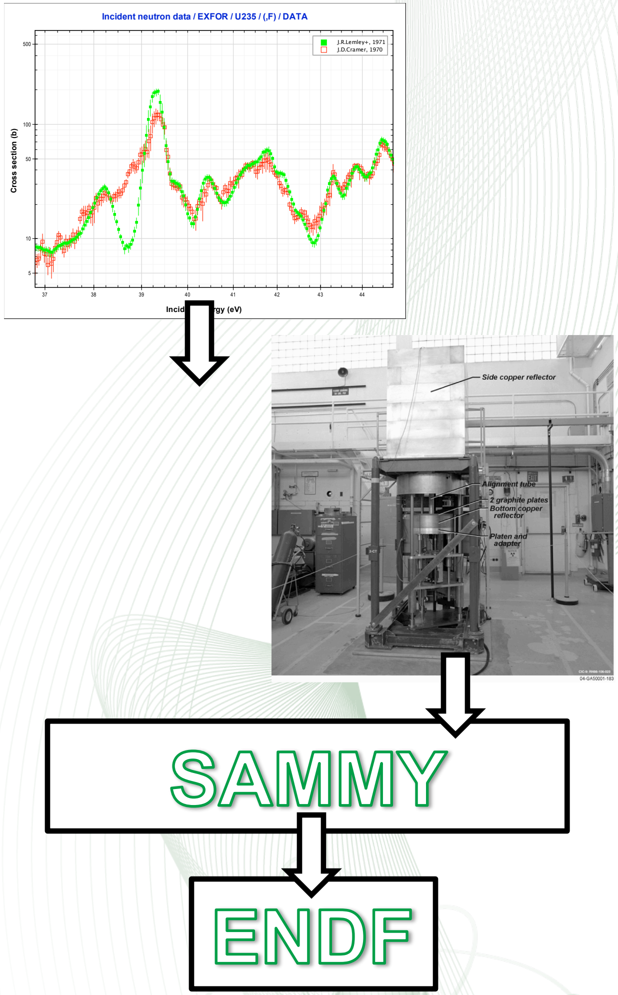


- Differential data → SAMMY → $d\sigma(E)/dP$ → SAMINT
- Integral data → CE TSUNAMI / MCNP-6 → $dk/d\sigma(E)$ → SAMINT
- SAMINT → dk/dP → SAMMY → Updated P and δP → ENDF

P stands for all resonance parameters: E_λ, Γ_γ, Γ_n, Γ_f, etc.

SAMINT Capabilities for Initial Release from RSICC

- 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 RSICC

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

Case Name	SAMINT Capability	Sensitivity Code	Notes
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 form appearance of zero cross-sections due to threshold reactions
tr183	- ^{239}Pu case - Fitting resonance parameter and nu-bar simultaneously - Independent eta updating	MCNP6	

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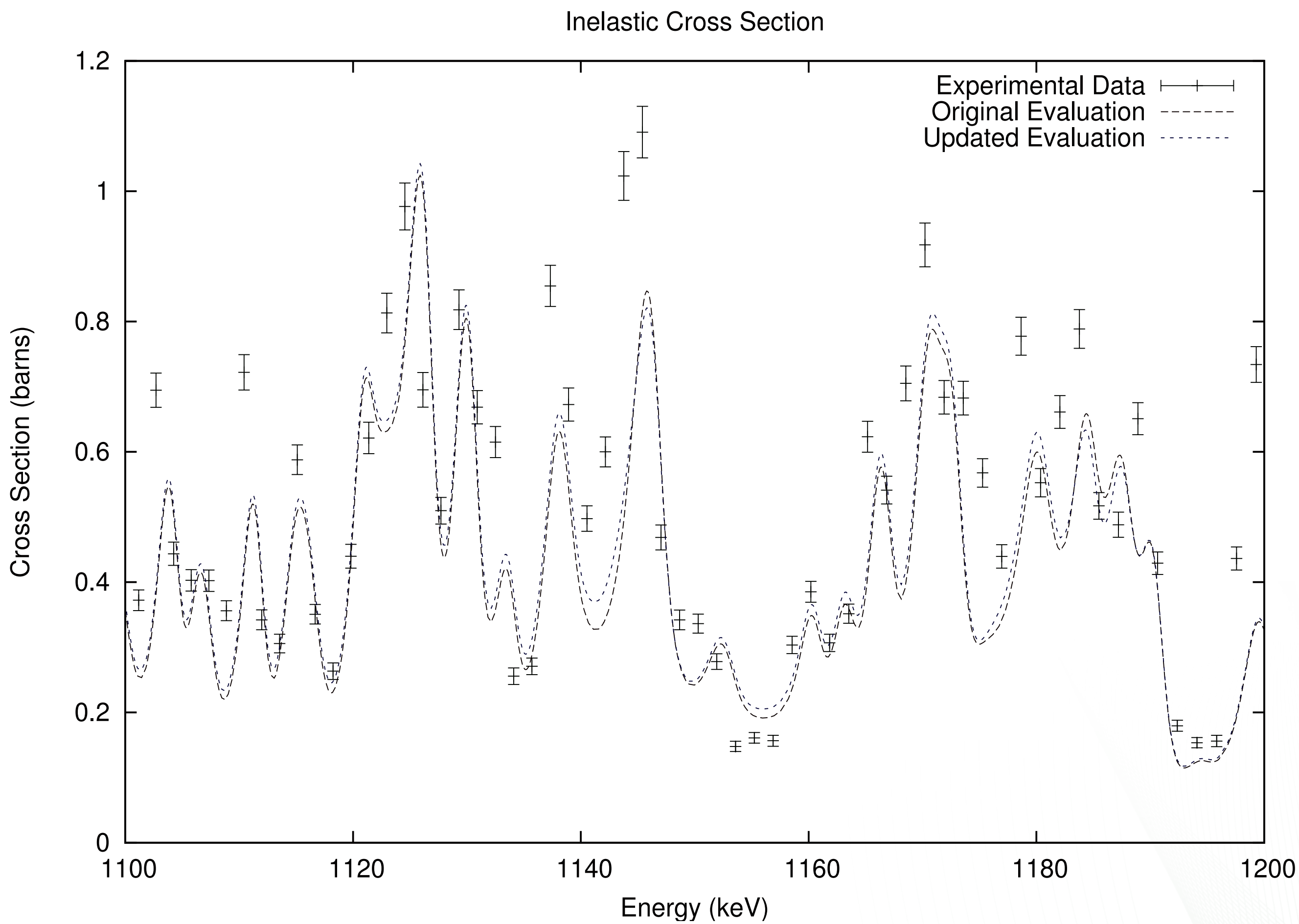
Sample Calculations

- 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:
  - Γ_{γ}: 450 keV – 2MeV
  - $\Gamma_{(n,n'),1}$ and $\Gamma_{(n,n'),2}$: 846 keV – 2MeV

Cross Section Changes:
Finer Scale than Differential Experimental Data



Inelastic cross section of ^{56}Fe before (χ^2 = 73.3382) and after (χ^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.

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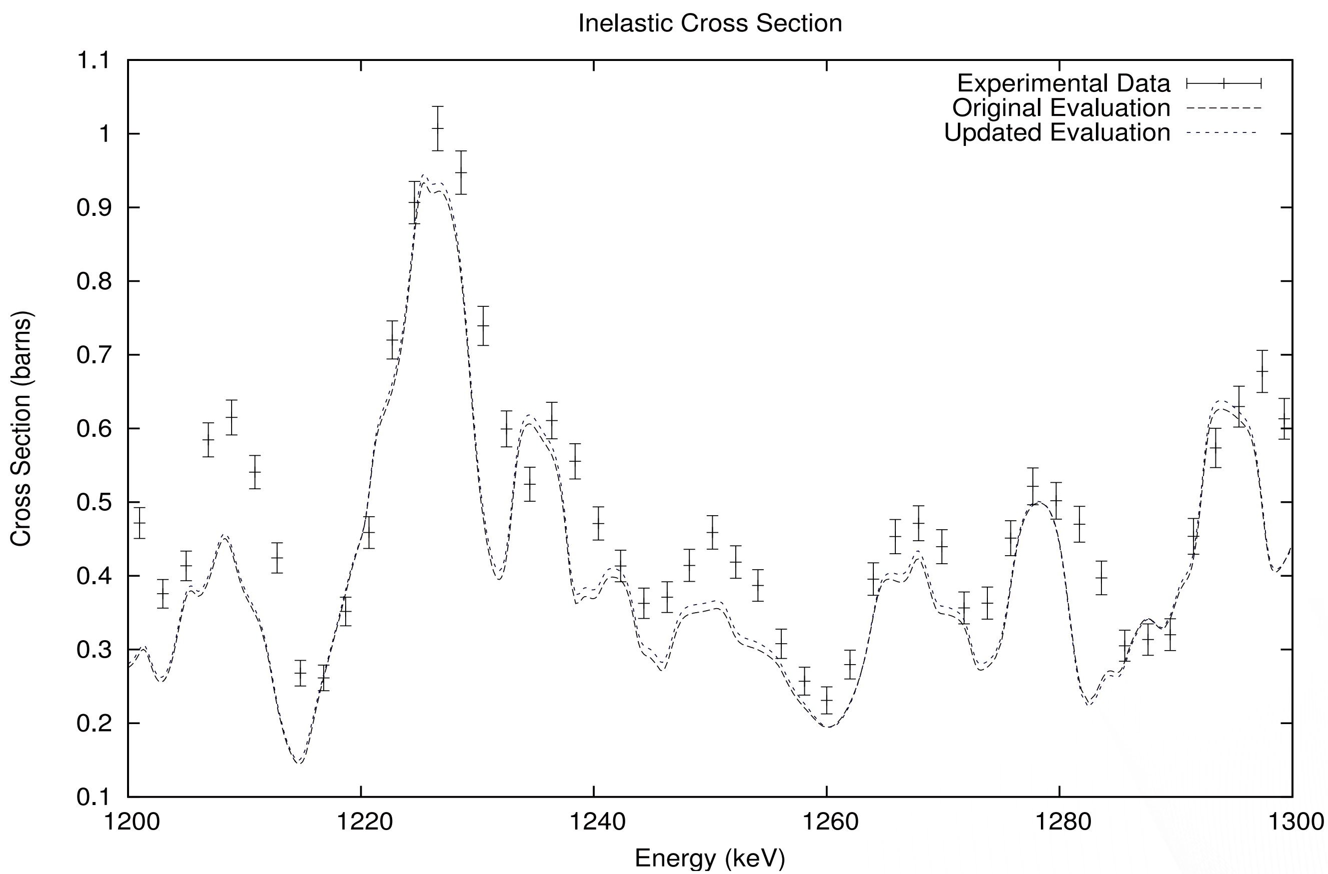
Cross Section Changes: Finer Scale than Differential Experimental Data



Inelastic cross section of ^{56}Fe before (χ^2 = 23.6023) and after (χ^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.

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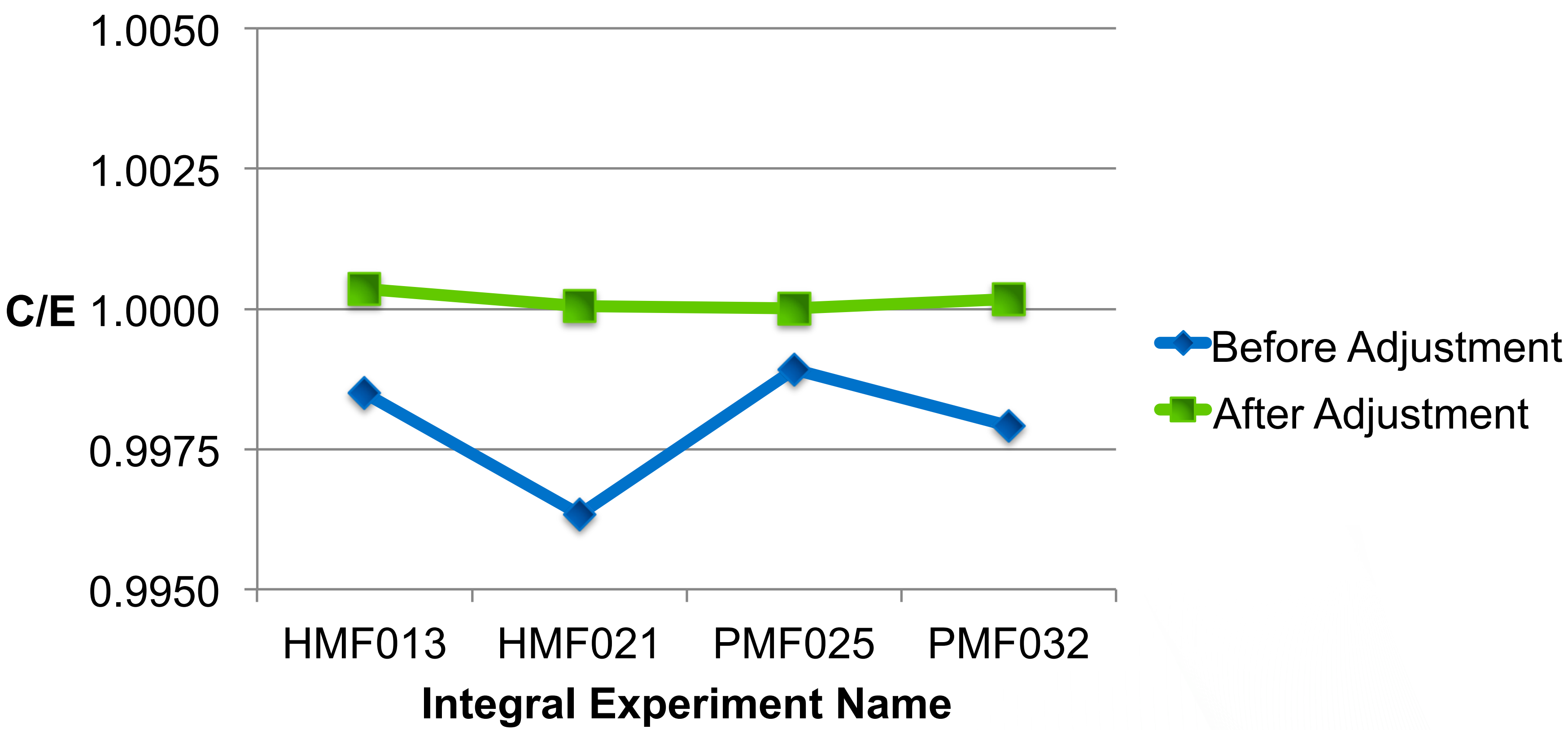
^{56}Fe Results



- **C/E**: $\dfrac{\text{Computed Value}}{\text{Experimentally Measured Value}}$

Expanded Capabilities

First Update Release (Spring)

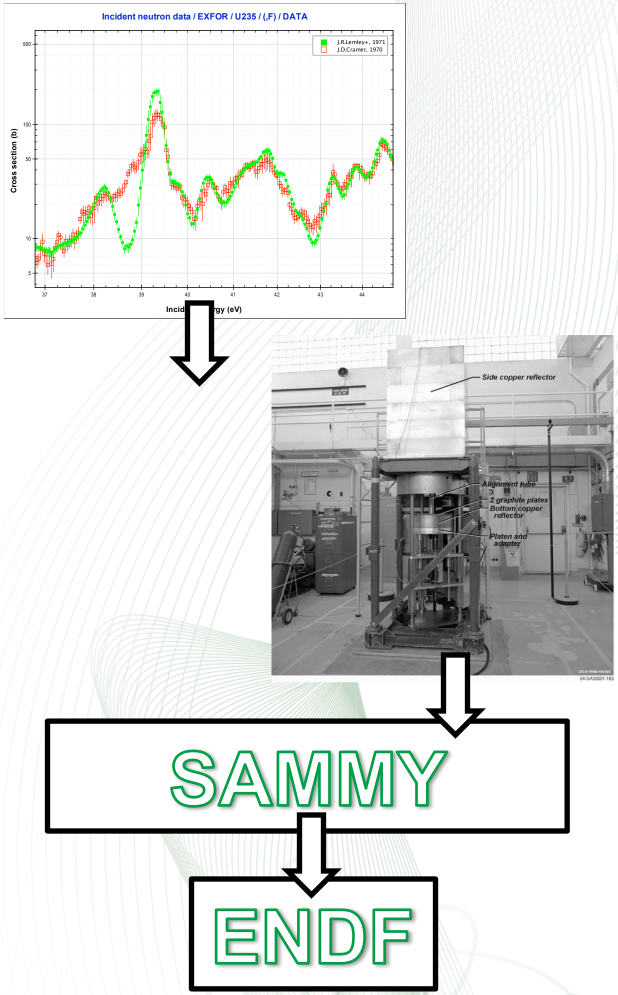
- Cross-Isotope correlation matrices
  - Determine the posterior correlation matrix created by adjusting several isotopes simultaneously
- Use of Angular Distribution Sensitivity with MCNP6 for adjusting resonance parameters
- Immediate application: ^{63}Cu and ^{65}Cu

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.



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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

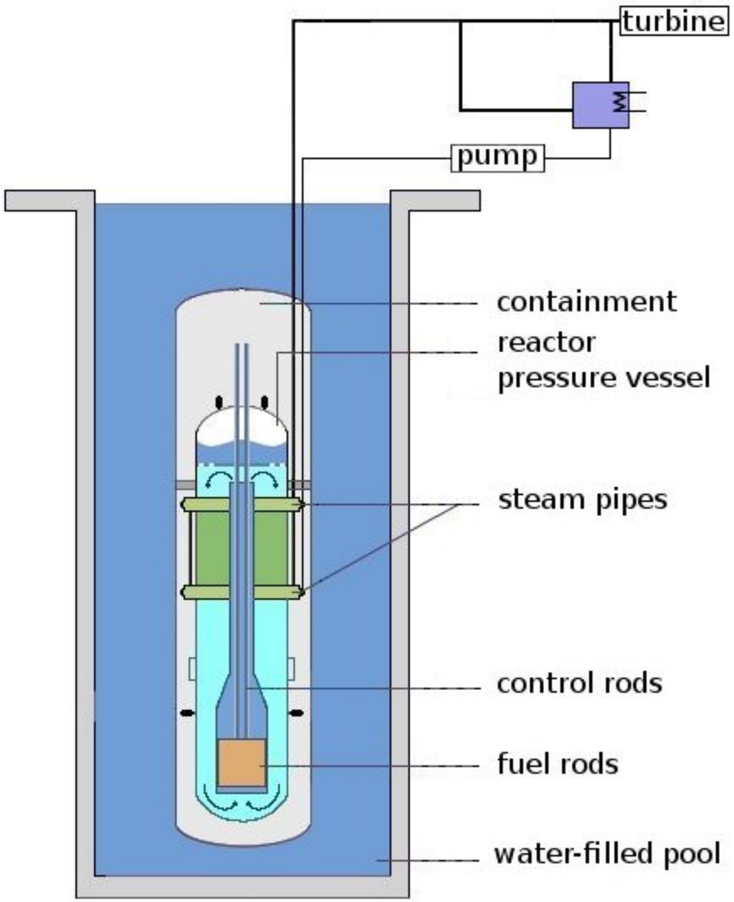
Applications

<u>Application Examples:</u>

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

<u>Response Examples</u>

- Neutron multiplication factor
- Cycle length
- Power distribution
- Reaction rate ratio



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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.:

$$\sigma_0 \pm \Delta\sigma_0 \Rightarrow R_0 \pm \Delta R_0 \text{ where } \Delta R_0 > \Delta R$$

- Inverse S/U: What set of improved data would lower the response uncertainty below the specified tolerance?
  - While minimizing the cost of data measurements

$$\sigma' \pm \Delta\sigma' \Rightarrow R' \pm \Delta R' \leq \Delta R \text{ for } \min(\text{cost}[\Delta\sigma'])$$

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:

$$\min\{\mathrm{Cost}[\Delta\sigma]\} \text{ such that}$$

$$S(\Delta\sigma)^2 S^T \leq (\Delta R)^2$$

$$S = \left.\frac{\delta R(x)}{\delta\sigma}\right|_{\sigma=\sigma_0}$$

- This is a constrained optimization problem:
  - MINCON: open source subroutine is used by MATLAB and DAKOTA

Including Integral Benchmark Experiments in IS/U

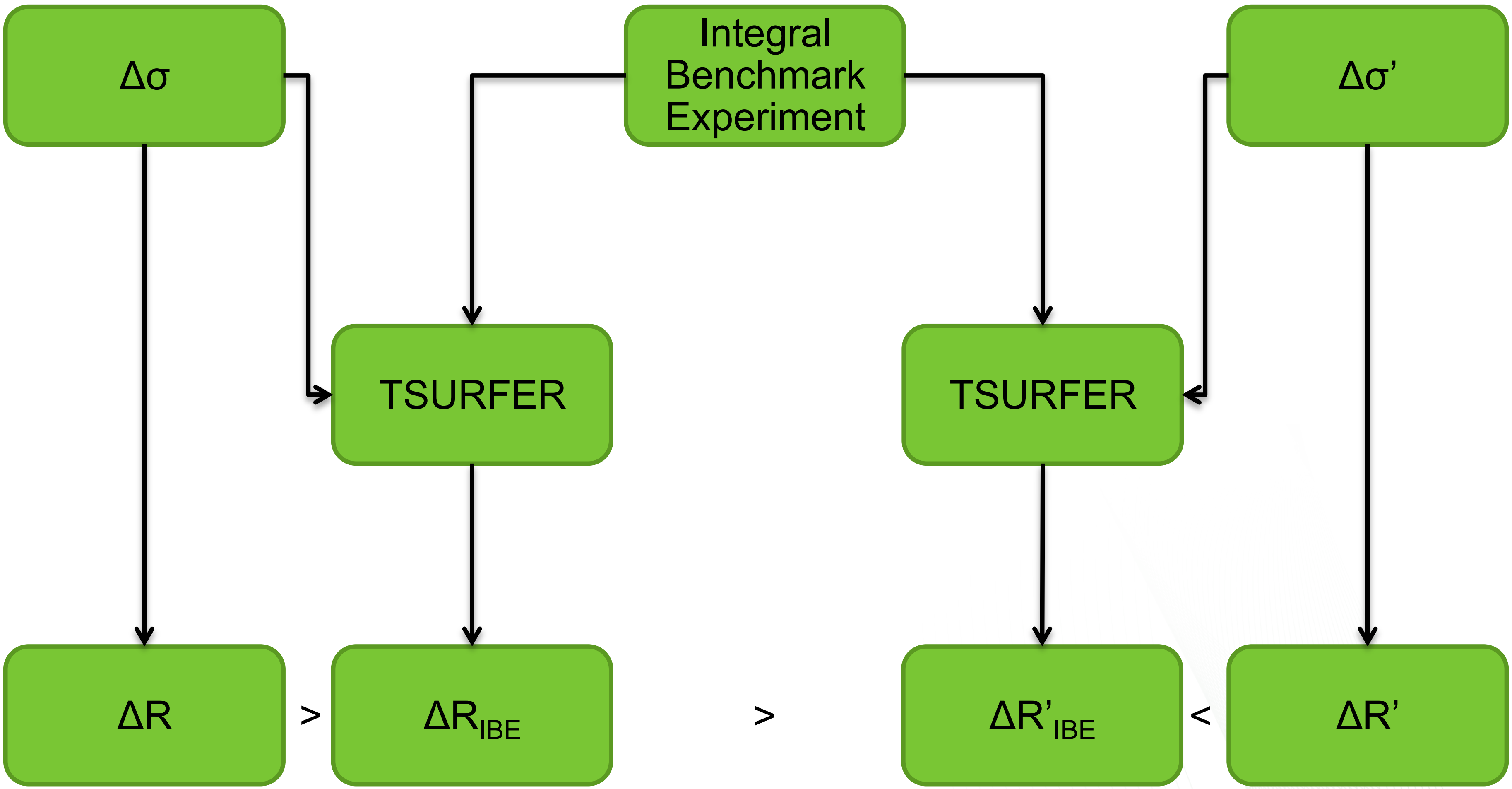
- Differential data uncertainties are limited by experimental methods
- Some data already at the present-day limits of experimental precision
- Uncertainties required by IS/U lower than these may be unrealistic

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

Reaction	*MT*	*Min. Rel. Uncertainty*
Fission	18	0.7%
Capture	102	2%
Neutron yields	452	0.3%
Elastic scattering	2	2%

- 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



Example Calculations

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

TABLE I. SUMMARY OF INVERSE S/U RESULTS

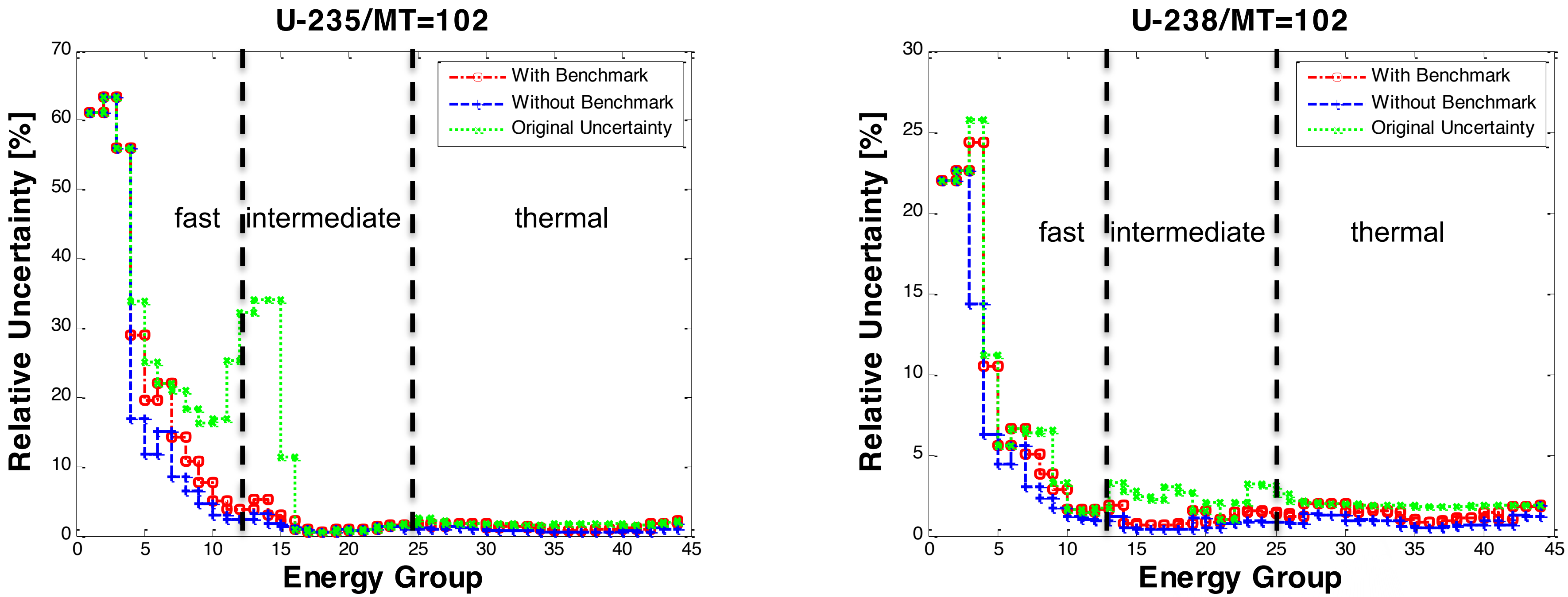
	w/o Benchmark	*w/Benchmark*
Cost (arb.)	53.3	8.6
$\mathrm{var}(k_{\mathrm{eff}})$	1.0E-06	1.0E-06

- 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

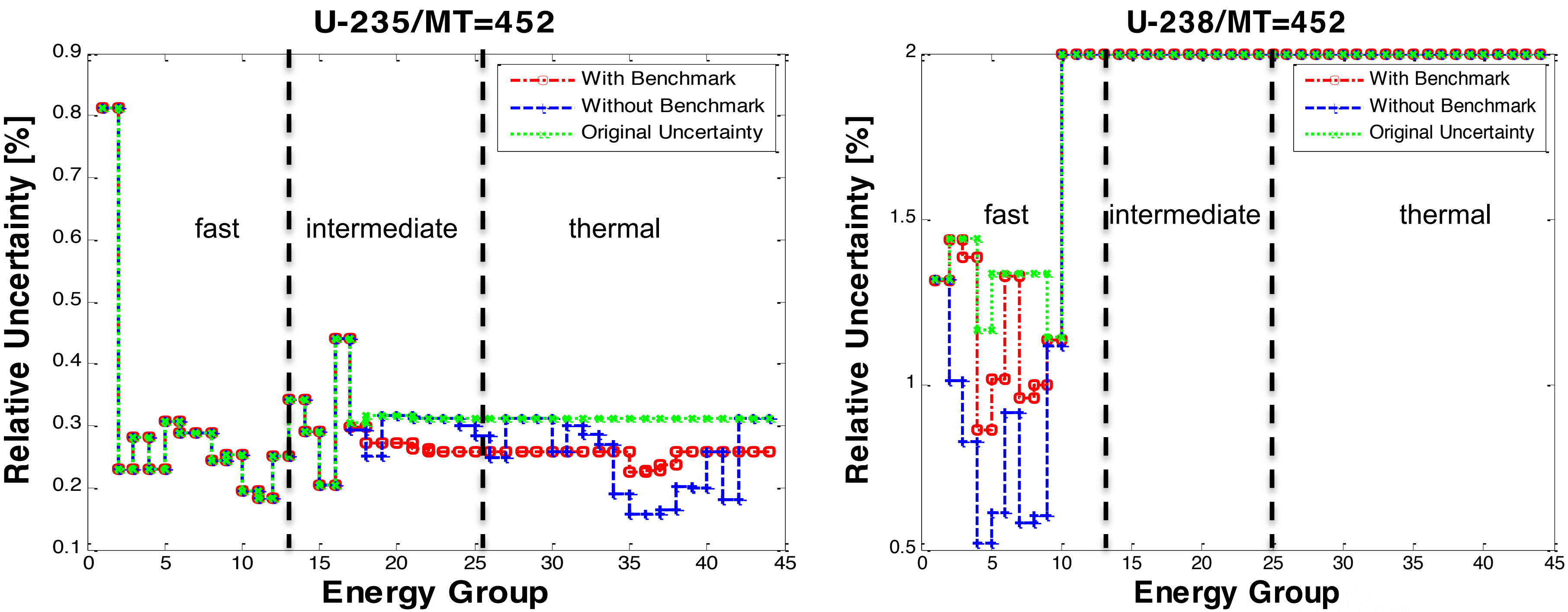
- So far, the cost of a differential experiment has been assumed to be inversely proportional with the uncertainty in the differential data
- A realistic cost function would account for
  - duration of measurements
    - Needed to run the facility, pay the staff, etc.
    - Inversely proportional to 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

Inverse S/U Results



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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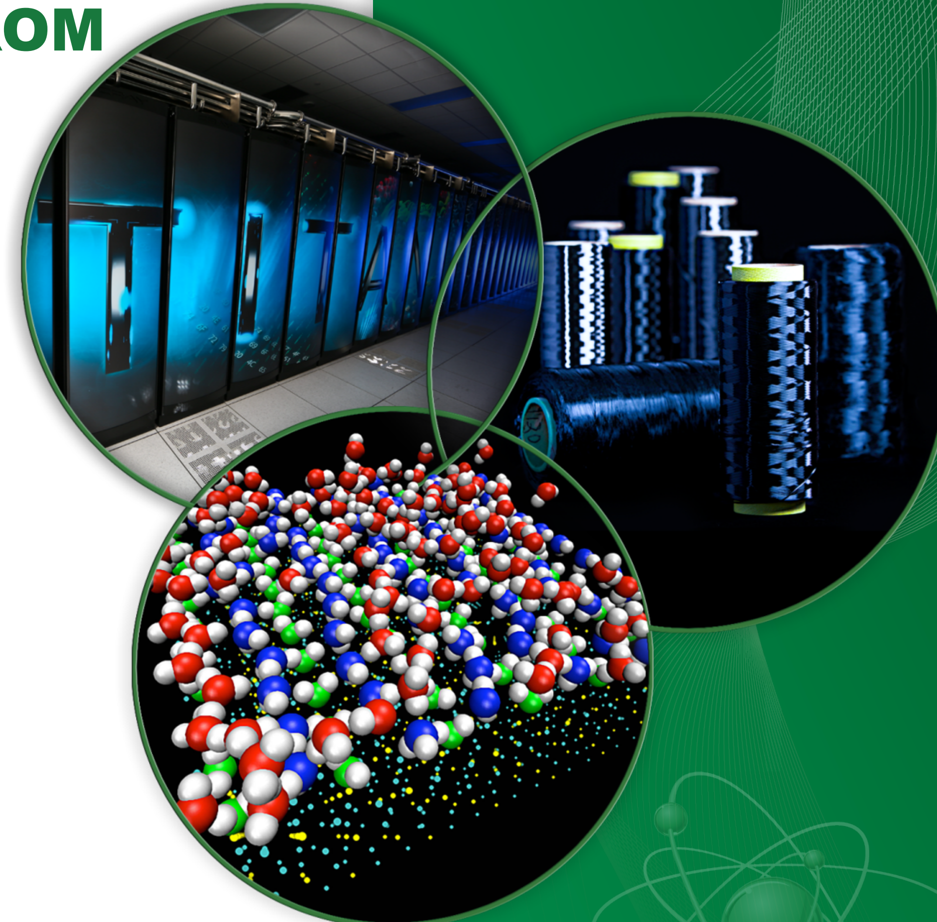

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