ORNL Cross-Section Covariance Processing Capabilities

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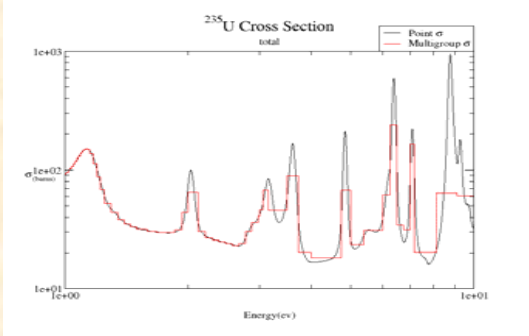
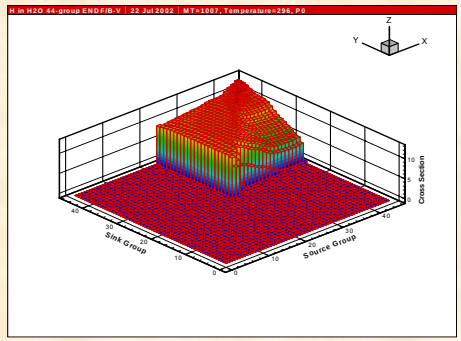
AMPX Cross-Section Processing System

- Process ENDF/B Formats
  - Generate Temperature-Dependent Pointwise Cross Sections
  - Provide Resonance Self-Shielding for RRR and URR
  - Probability Table Generation for URR
  - Energy and Angle Distributions for Secondary Particles
  - Process S(α,β) Data for Thermal Moderators
  - Generate free-gas S(α,β) Data for Non-Thermal Moderators
  - Process Particle-Yield Data
  - Generate Pointwise Weighting Spectra
  - Multigroup Averaging Operations
  - **Process Cross-Section Uncertainty Data for Use in Sensitivity/Uncertainty (S/U) Methods**
  - Automated Cross-Section Library Production—Process Multiple Nuclides





- SCALE relies on nuclear data and processing procedures from AMPX:
  - Multigroup (MG) and continuous-energy (CE) cross-section data
  - Data processing procedures including problem-dependent resonance self-shielding
  - Cross-section uncertainty data to support S/U methods in SCALE

Covariance Data Processing Improvements

PUFF-IV Module Development for AMPX code system

- Complete rewrite of PUFF-III code in F90.
- Results are the same as in PUFF-III within rounding errors
- Automatic test cases comparing PUFF-III results and PUFF-IV results
- Processes ENDF/B Files 31, 32 and 32
- Utility modules available to interface with NJOY-generated libraries

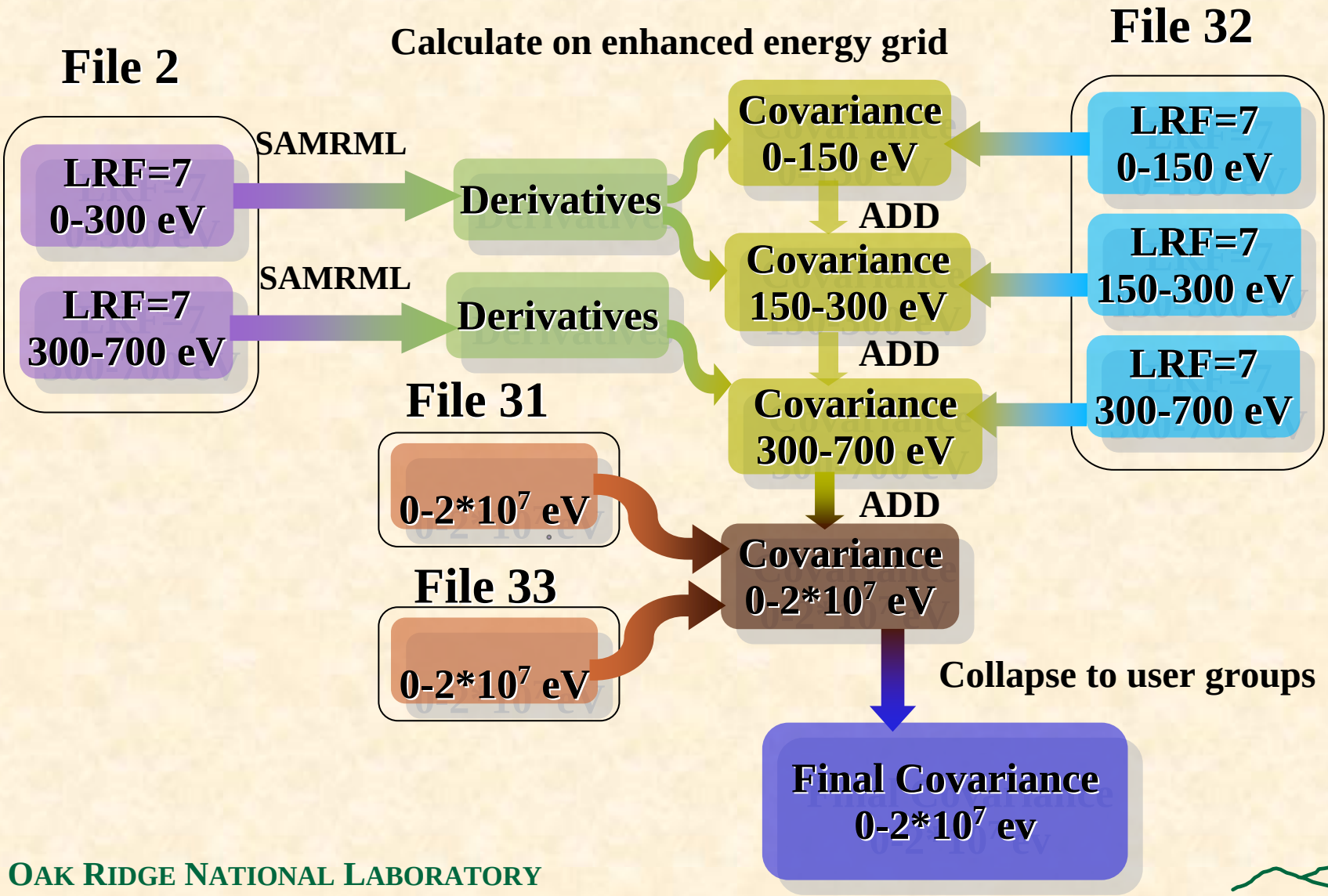
File 32 resonance parameter covariance processing

- Derivatives are calculated from File 2 using SAMRML
- Group averages of covariances are calculated using the above derivatives
- Resolved region data can be handled—existing ENDF/B unresolved formats can be processed
- Resolved region: lrf=1,2,3 and lcomp=0,1,2, lrf=7 and lcomp=2
- Internal test cases to ensure proper working of group averaging
- Automatic test cases to compare results with SAMMY generated group averaged covariance data

PUFF-IV standalone package delivered to RSICC for testing and distribution
Release expected in next few weeks

- Testing performed with ENDF/B-VII Beta 2, ENDF/B-VI.8, ENDF/B-V
- Some testing performed with JEFF and JENDL evaluated data files

Example PUFF-IV Processing Flow Diagram



PUFF calculation of file 32 covariances

Cross section from file 2: $\sigma_m(E) = \sigma_m(E, P_j)$

The covariance for the parameters is: $Cov(P_i, P_j) = \langle \delta P_i ; \delta P_j \rangle$

The propagated covariance for cross section:

$$\langle \delta\sigma_m(E_i)\delta\sigma_l(E_j) \rangle = \left\langle \sum \frac{\partial\sigma_m(E_i)}{\partial P_k}\delta P_k \sum \frac{\partial\sigma_l(E_j)}{\partial P_n}\delta P_n \right\rangle$$

$$= \sum \frac{\partial\sigma_m(E_i)}{\partial P_k} \langle \delta P_k \delta P_n \rangle \frac{\partial\sigma_l(E_j)}{\partial P_n}$$

Group averaged covariance:

$$\langle \delta x_I^m \delta x_J^l \rangle = \frac{1}{\Phi_I \Phi_J} \int \Phi(E_i) \langle \delta\sigma_m(E_i)\delta\sigma_l(E_j) \rangle \Phi(E_j) dE_i dE_j$$

Separating the integral and substituting a sum for the integral

$$\langle \delta x_I^m \delta x_J^l \rangle = \sum D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l$$

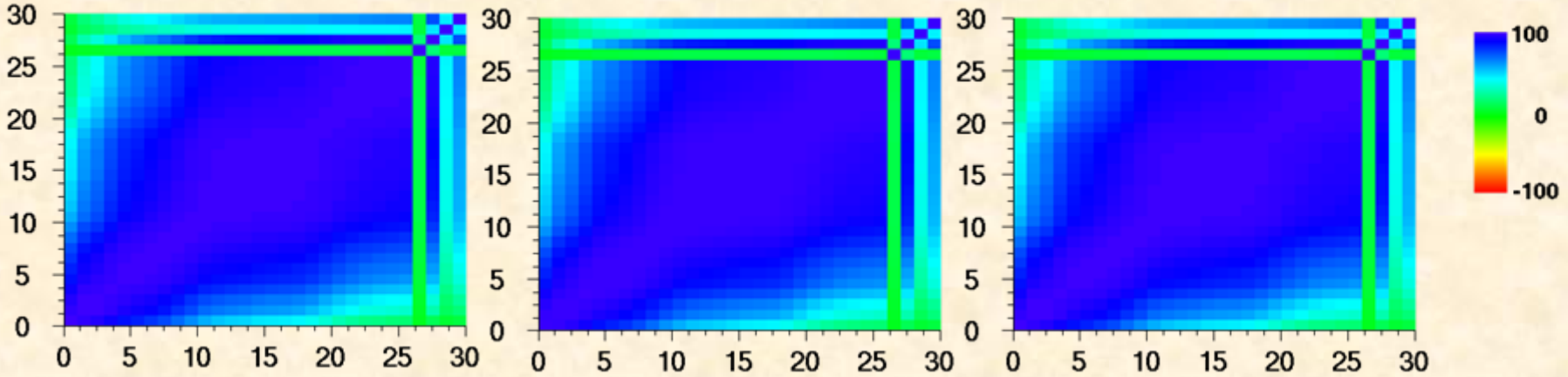
with $\Phi_I = \sum \Phi(E_i) \Delta E_i$ and $D_{Ik}^m = \frac{1}{\Phi_I} \sum \Phi(E_i) \frac{\partial\sigma_m(E_i)}{\partial P_k} \Delta E_i$

^{158}Gd resolved region only: Total cross section – flat flux

JENDL-3.2, for comparison with Errorj: lrf=3, lcomp =1

Correlation matrices

Sammy **Puff-IV** **Errorj**



Std. deviation

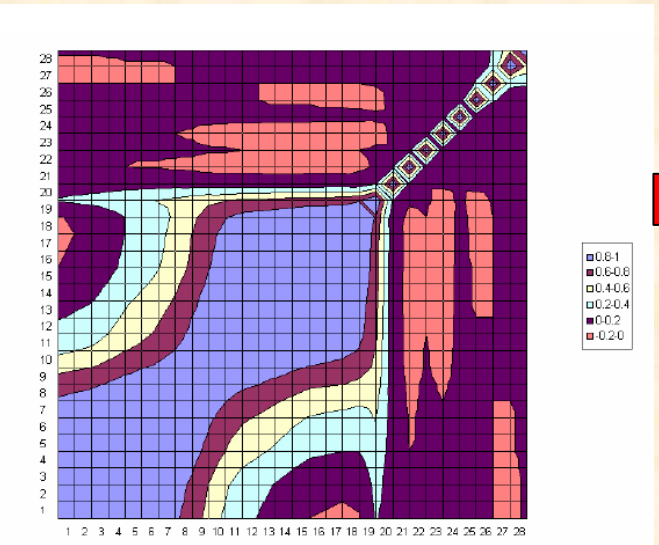
Largest absolute difference:

Errorj -Sammy: $1.21*10^{-5}$

Errorj -Puff-IV: $5.22*10^{-6}$

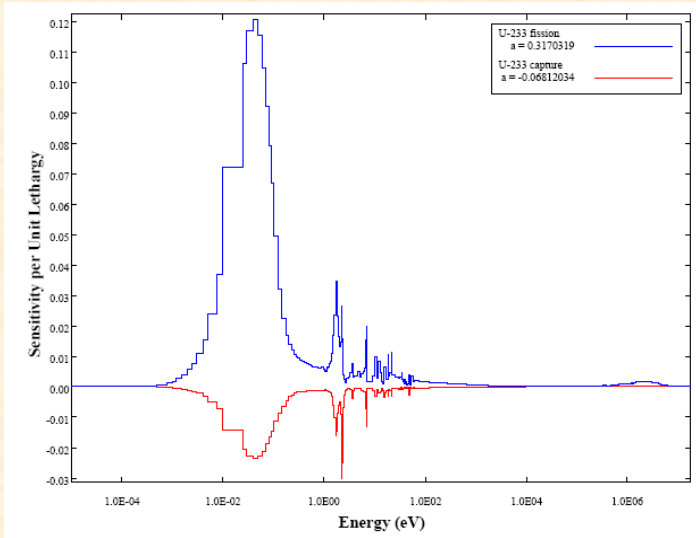
Sammy - Puff-IV: $1.30*10^{-5}$

^{233}U Covariance Data for Criticality Applications

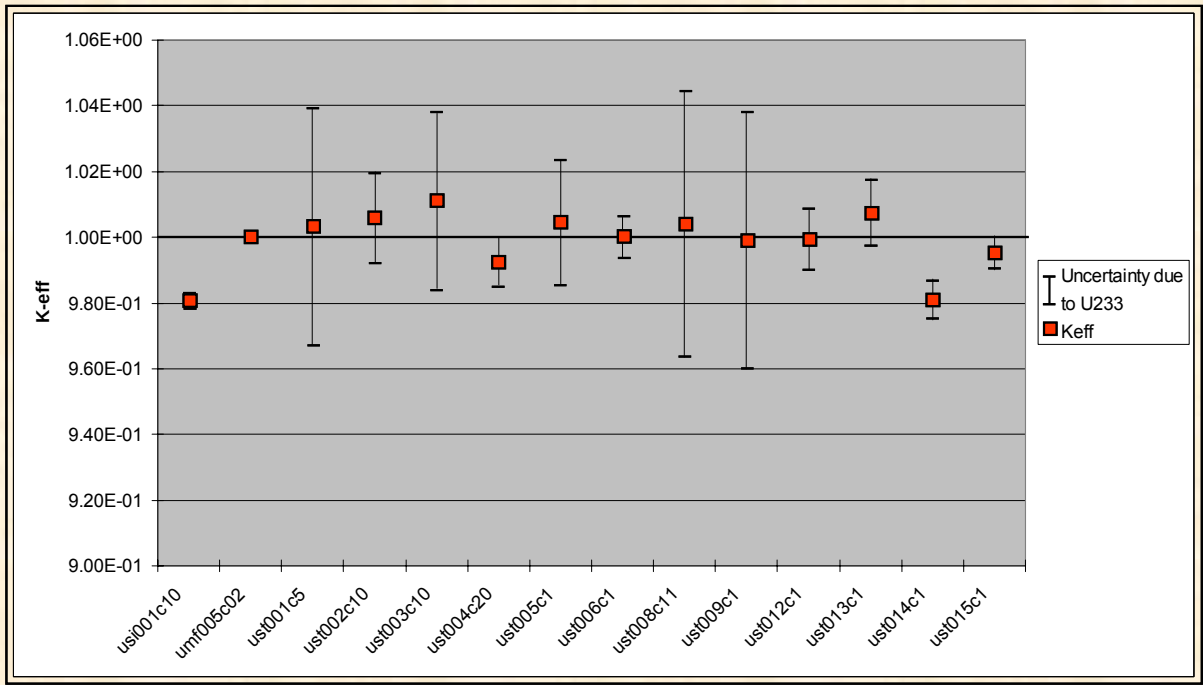


PUFF-IV
^{233}U
Covariance
Data

SCALE
TSUNAMI
Sensitivity/
Uncertainty
Analysis



Propagation of
Cross-section
Covariance
Data to k_{eff}



R&D Recommendations

- AFC Workshop emphasize need for covariance data
- Nuclear Data community needs to produce evaluated covariance data
  - Covariance evaluation methods are still evolving
  - New covariance ENDF/B covariance formats will be developed—unresolved region
- **Need to develop and maintain covariance processing capabilities to keep pace with new evaluation capabilities**
- Invest in processing methods to maintain bridge between nuclear data evaluations and applications—otherwise new data evaluations will not be useable