AMPX Covariance Processing Status

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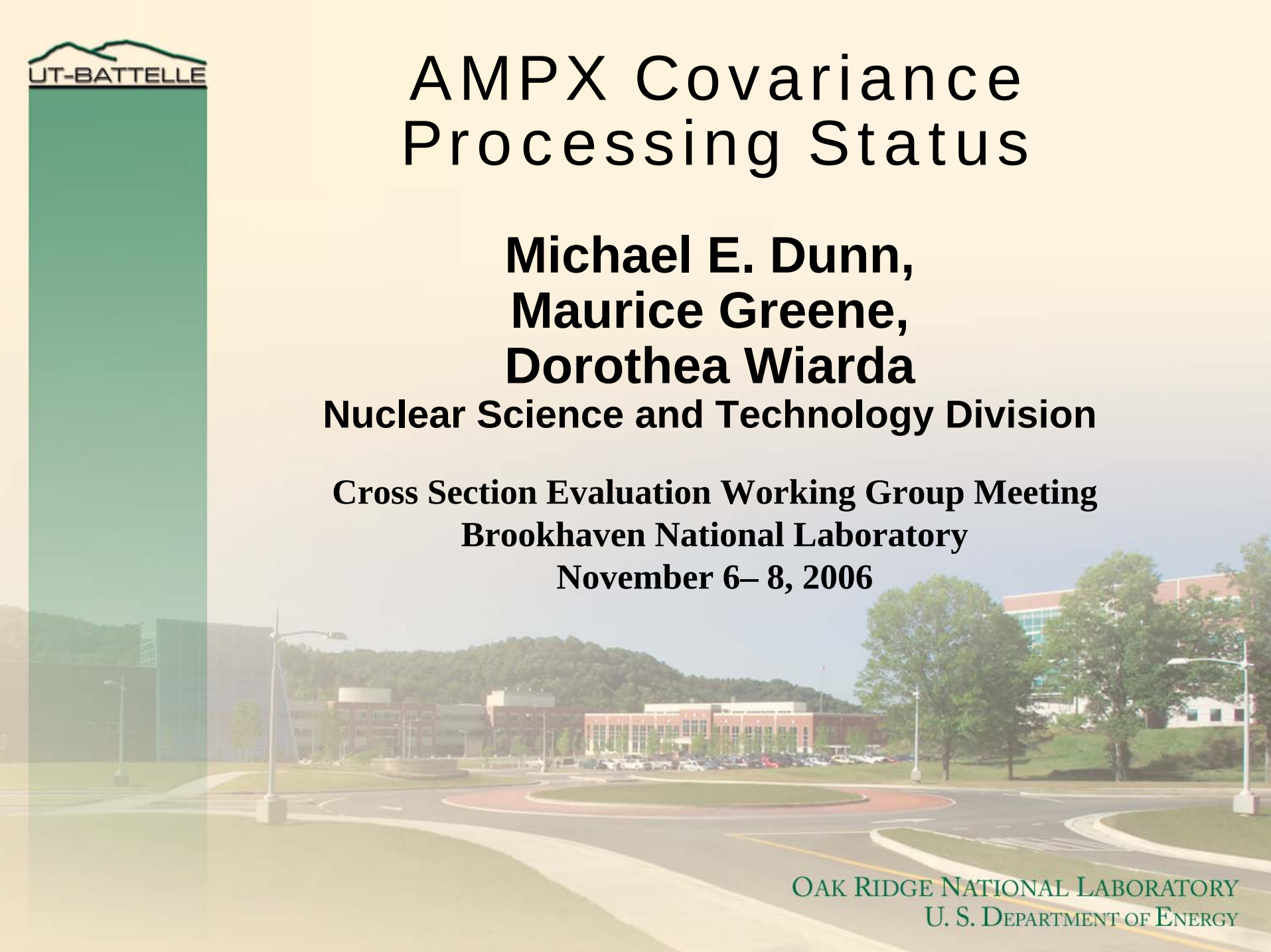
Cross Section Evaluation Working Group Meeting
Brookhaven National Laboratory
November 6– 8, 2006



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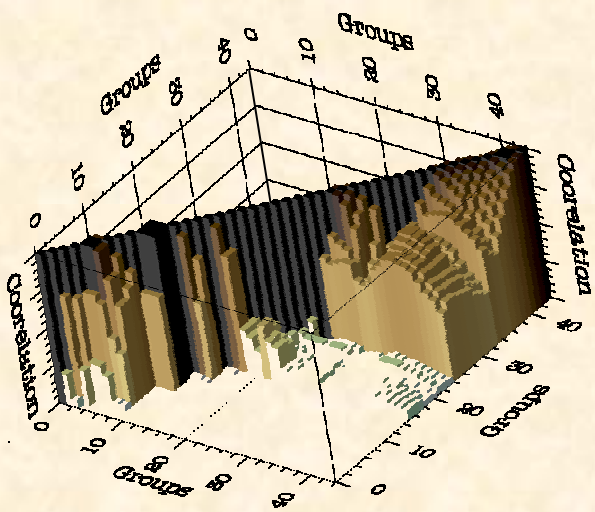
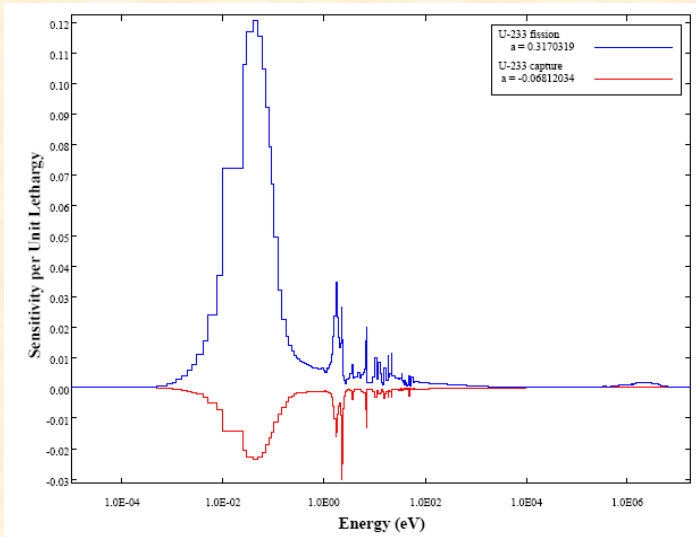
AMPX Covariance Data Processing

- PUFF-IV processes ENDF uncertainty data and generates multigroup covariance and correlation matrices for a user-specified energy structure
- Process ENDF data through version VII
- Developed for implementation in the AMPX Cross-Section Processing System.
- Covariance data are saved in COVERX format
- Cross-Section uncertainty data from PUFF-IV can be propagated through sensitivity studies to final calculated quantity of interest





SCALE TSUNAMI Sensitivity/ Uncertainty Analysis

Covariance Data Processing Improvements

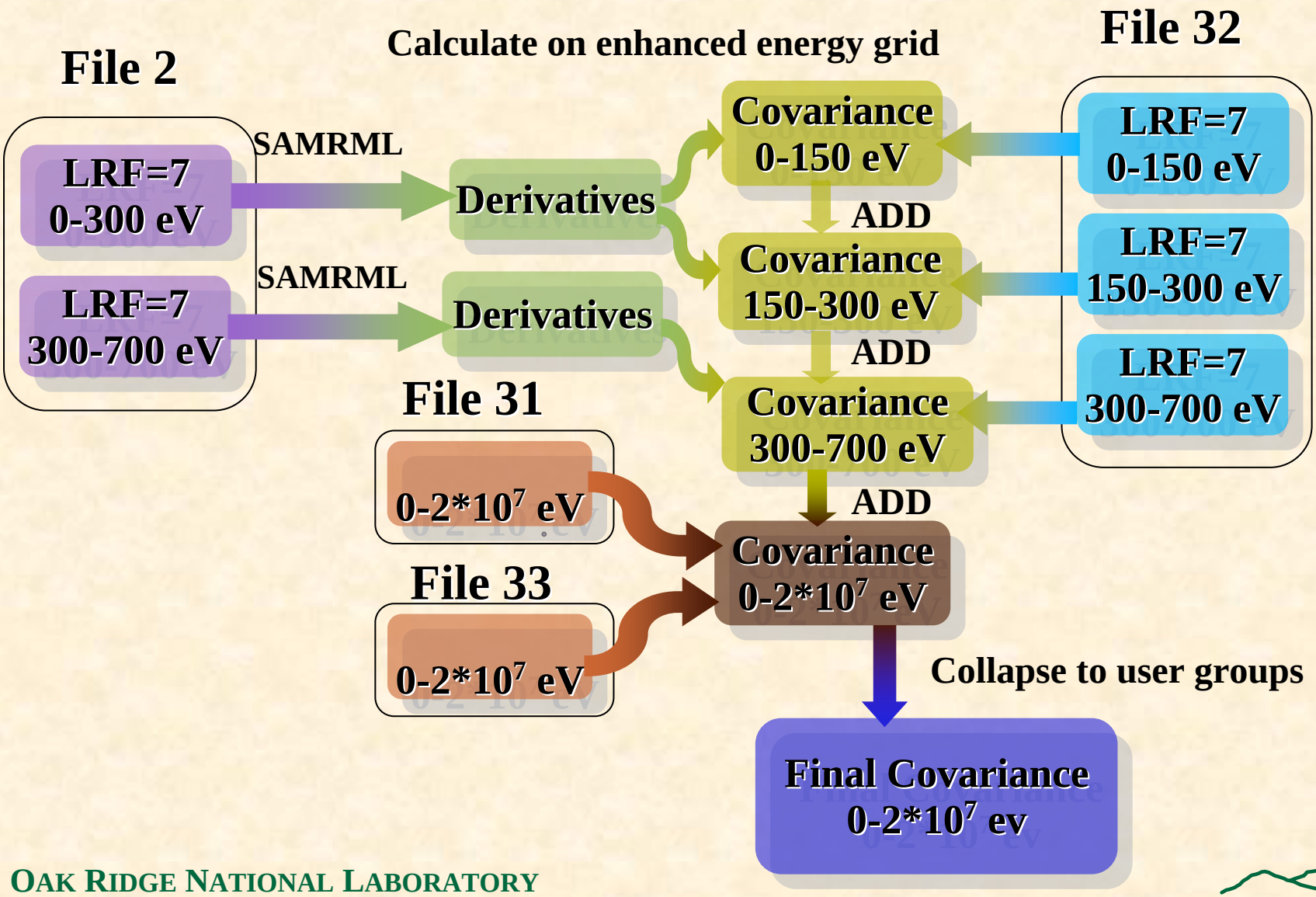
PUFF-IV Module Development for AMPX

- Complete rewrite of PUFF-III code in F90.
- Object oriented design as far as possible in F90
- Process ENDF/B Files 31, 32 and 33
- Results are the same as in PUFF-III within rounding errors
- Automatic test cases comparing PUFF-III results and PUFF-IV results
- Utility capabilities to interface with NJOY MG libraries and compare COVERX formatted covariance files

File 32 processing

- Derivatives are calculated from File 2 using SAMRML
- Group averages of covariances are calculated using the above derivatives
- Resolved and unresolved region data can be handled
- Resolved region: lrf=1,2,3 and lcomp=0,1,2, lrf=7 and lcomp=2 (lrf=1,2 resonance parameters are translated to Reich-Moore formalism before calculating derivatives)
- Internal test cases to ensure proper working of group averaging
- Automatic test cases to compare results with SAMMY generated group averaged covariance data

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

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

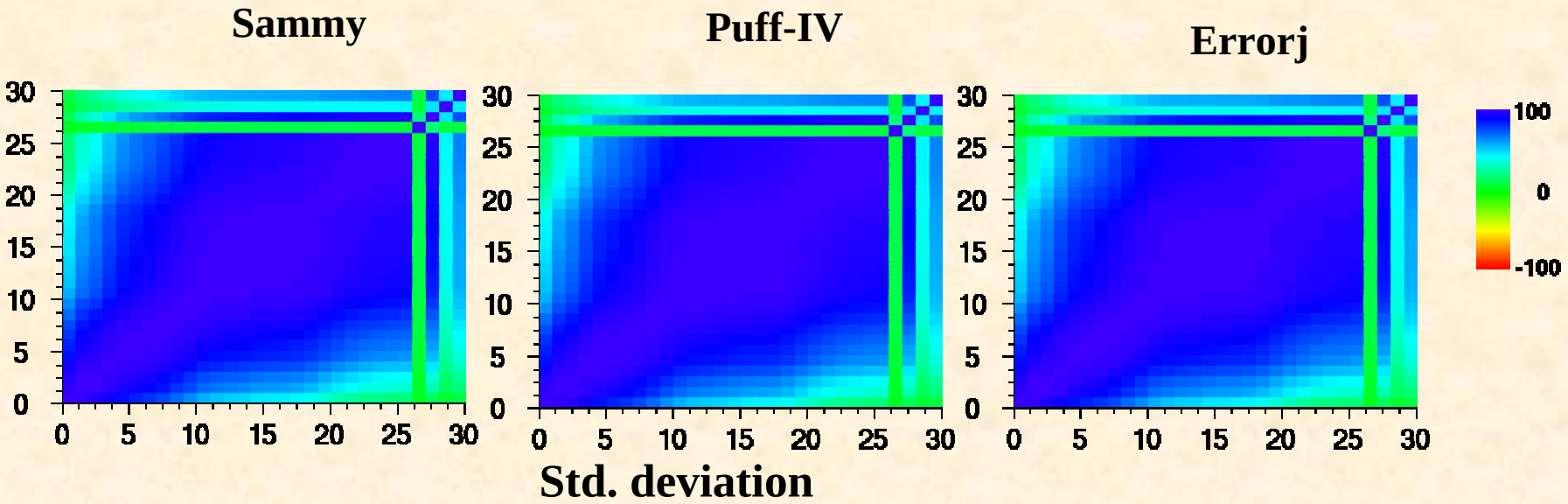
with $\Phi_I = \sum \Phi(E_i) \Delta E_i$ and $D_{Ik}^m = \frac{1}{\Phi_I} \sum \Phi(E_i) \frac{\partial\sigma_m(E_i)}{\partial P_k} \Delta E_i$

PUFF-IV Covariance Data Processing Examples

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

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

Correlation matrices



Largest absolute difference:

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

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

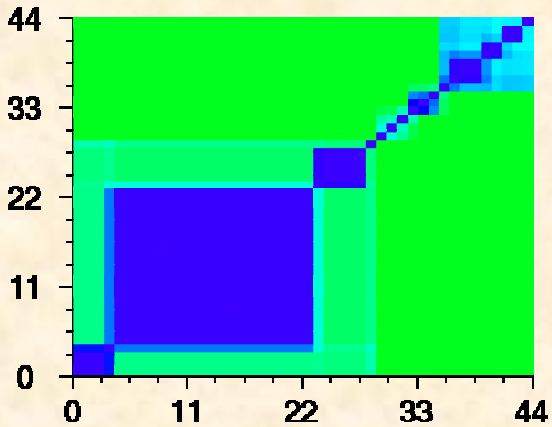
Sammy - Puff-IV: $1.30*10^{-5}$

PUFF-IV Covariance Data Processing Examples

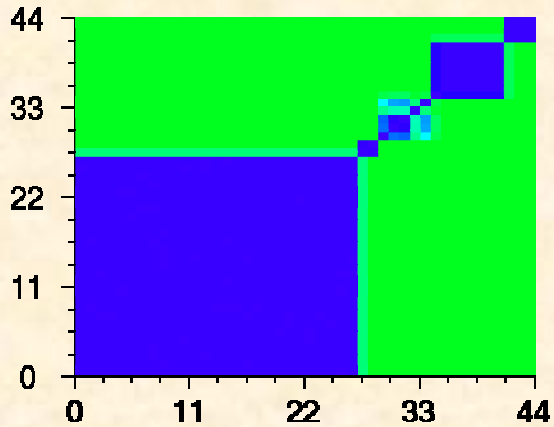
^{23}Na: File 33 and File 32 processing – flat flux

ENDF/B-VI MOD2
lrf=2, lcomp=0
Sensitivity analysis for File 32
Puff-III and Puff-IV (identical results)

Total cross section



Capture cross section



Comparison between ENDF-VIIB2 and ENDF-VIIB3 covariance data

PUFF-IV was run on all ENDF files containing File 31, 32 and/or 33 data. Results of Beta 2 and Beta 3 data are compared using COVCOMP, which compares relative covariance matrix data.

- Unchanged between Beta 2 and Beta 3
  ^{6}Li std., 10B, ^{19}F, ^{23}Na, ^{48}Ti, V, ^{59}Co, ^{58}Ni, ^{93}Nb, ^{156}Gd, ^{158}Gd, ^{160}Gd, ^{197}Au, 197Au std., ^{209}Bi, ^{235}U std., ^{238}U std.

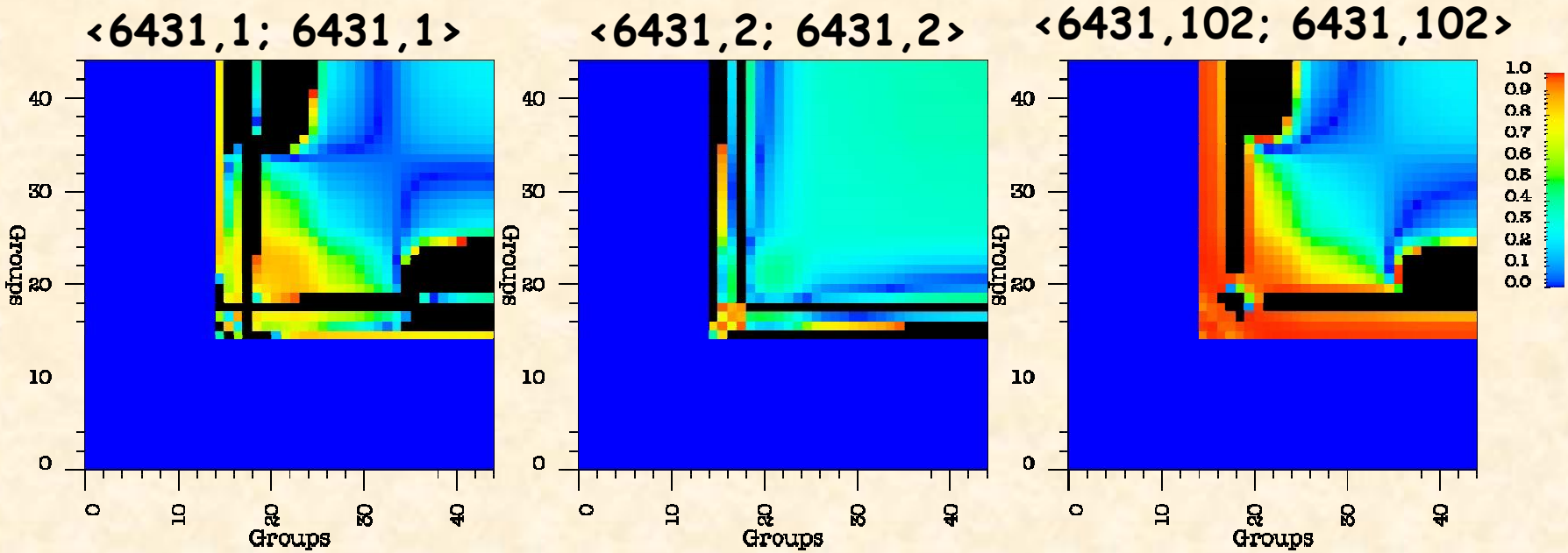
- Added in Beta 3
  ^{10}B std., ^{89}Y, ^{99}Tc, ^{191}Ir, ^{193}Ir

- Changed between Beta 2 and Beta 3
  ^{6}Li, ^{152}Gd, ^{153}Gd, ^{154}Gd, ^{155}Gd, ^{157}Gd, ^{232}Th, ^{235}U

Gd isotopes

- Point-wise data as well as thermal values are used to determine the resonance parameters and corresponding covariance matrix.
- The uncertainty used for the thermal values changed between Beta 2 and Beta 3, thus changing the covariance matrix
- Affected isotopes:
  ^{152}Gd, ^{153}Gd, ^{154}Gd, ^{155}Gd ^{157}Gd

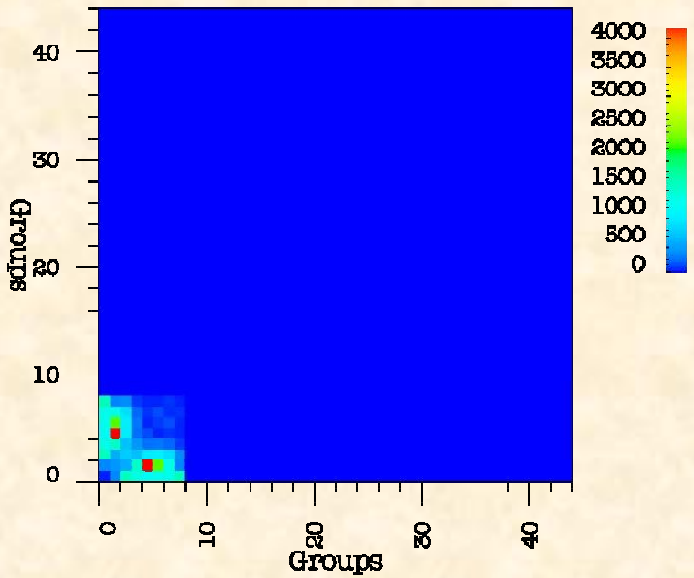
Relative difference >1: black. Largest difference: 180



^{232}Th, MAT=9040

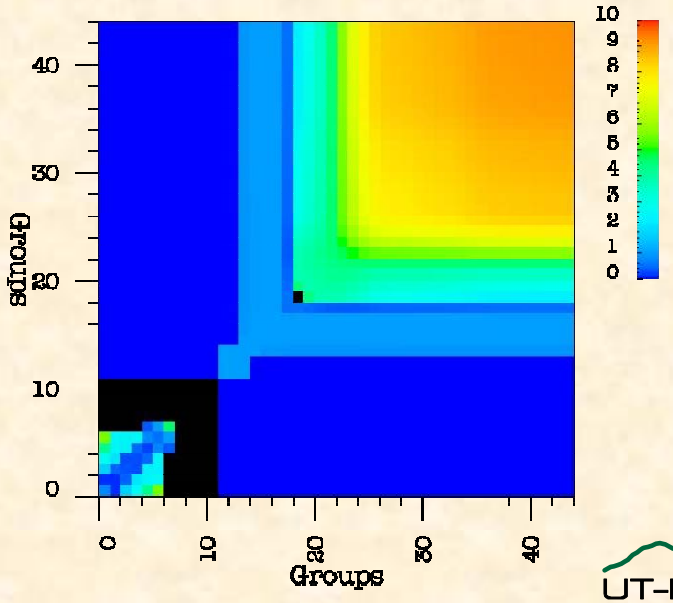
- Changes in resonance parameter covariances are due to changes in uncertainty in thermal values.
- References to ENDV-V numbers have been deleted
- Many cross reaction value covariances matrices are added in File 33
- All high energy covariances data in File 33 are different between Beta 2 and Beta 3.

<9040,854; 9040,854>



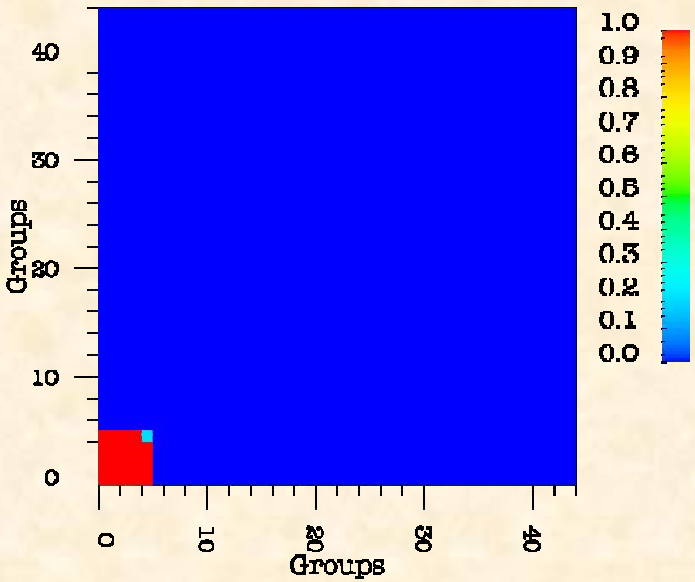
Relative difference >1: black.
Largest difference: 1200

<9040,102; 9040,102>



^{6}Li, MAT=325

- Only one covariance matrix <325,105;325,105> is given.
- In Beta 2 it was described by an LB=5 section
- Beta 3 adds an additional LB=1 section to cover a high energy range not covered by the LB=5 section.



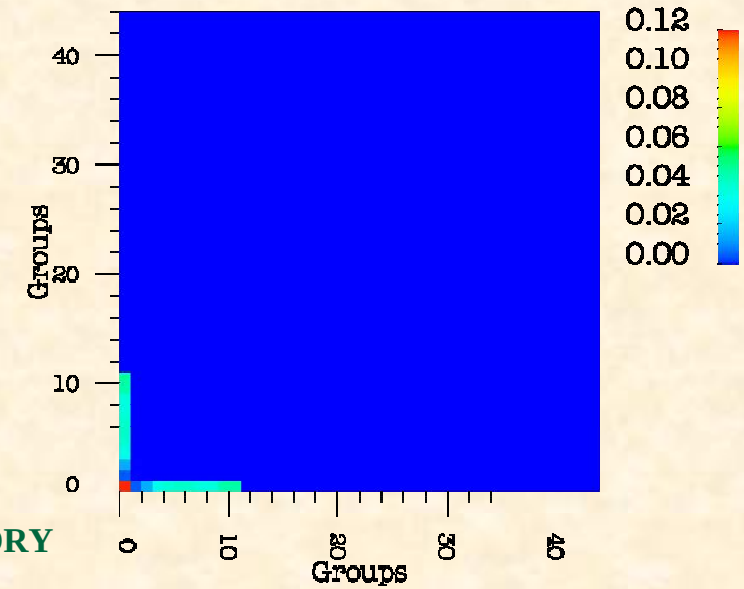
^{6}Li, MAT=325, standard file

- The new LB=1 section was not added in this file.
- Covariance matrix is unchanged between Beta 2 and Beta 3

^{7}Li, MAT=328

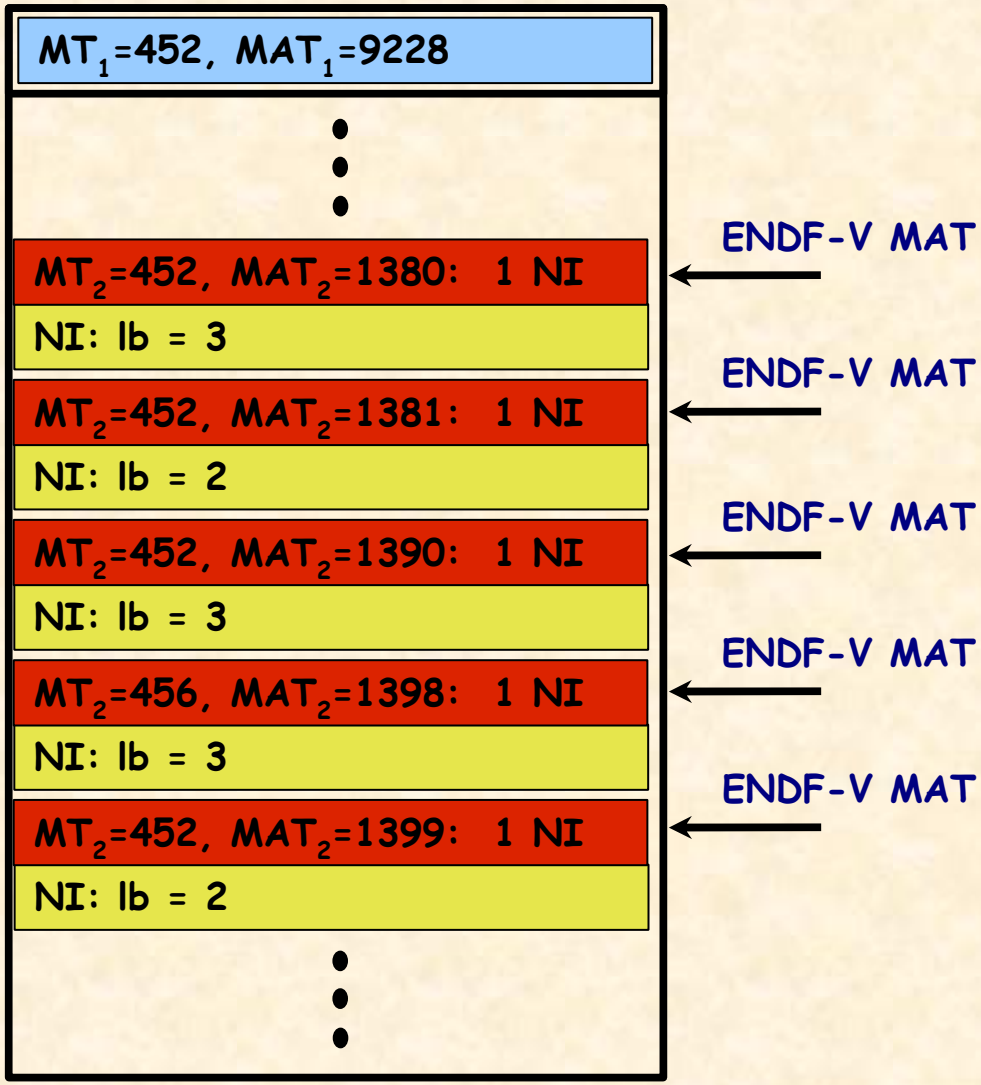
- Components for lumped reaction 851 have been added
- Many more covariances matrices are added in File 33. Among them <328,4; 328,851>.
- Explicit covariance matrices that appear in Beta 2 and Beta 3 are unchanged
- Covariance <328,2; 328,2> is affected by the change since it is given as an NC section, i.e. the cross section for MT=2 is calculated as a sum over cross sections MT=1, 4 and 851

<328,2; 328,2>



^{235}U, MAT=9228

^{235}U File 31 content



- References to ENDF-V numbers are used in File 31. This is unchanged from Beta 2 to Beta 3
- Cross section data in File 1 for MT=452 and MT=456 are changed in Beta 3.
- Since covariance data are given as relative matrices in File 33, covariance matrices are not affected by the change in cross section data.

ENDF-VII-B3 standard files

Standard files contain standard reaction covariance matrices. The same matrices are expected to be present in the neutron library files.

	Neutron library file	Standard file		
6Li	<MT=105;MT=105>	<MT=105;MT=105>	×	Matrices differ
C	-	<MT=2;MT=2>	×	
^{197}Au	<MT=1;MT=1>	<MT=102;MT=102>	×	
^{235}U	<MT=452; MT=452> <MT=456; MT=456>	<MT=18;MT=18>	×	
^{238}U	-	<MT=18;MT=18>	×	
^{10}B	<MT=800; MT=800> <MT=801; MT=801> <MT=800; MT=801> <MT=107; MT=107> <MT=107; MT=800> <MT=107; MT=801>	<MT=800; MT=800> <MT=801; MT=801> <MT=800; MT=801> <MT=107; MT=107> <MT=107; MT=800> <MT=107; MT=801>	*	

How to obtain PUFF-IV

Puff is available from RSICC at http://www-rsicc.ornl.gov

Radiation Safety Information Computational Center (RSICC)
P.O. Box 2008, Oak Ridge, TN 37831-6362 USA

The PUFF-IV package Code Number:
P00534.