AMPX Cross-Section Processing Status

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Cross Section Evaluation Working Group Meeting
Brookhaven National Laboratory
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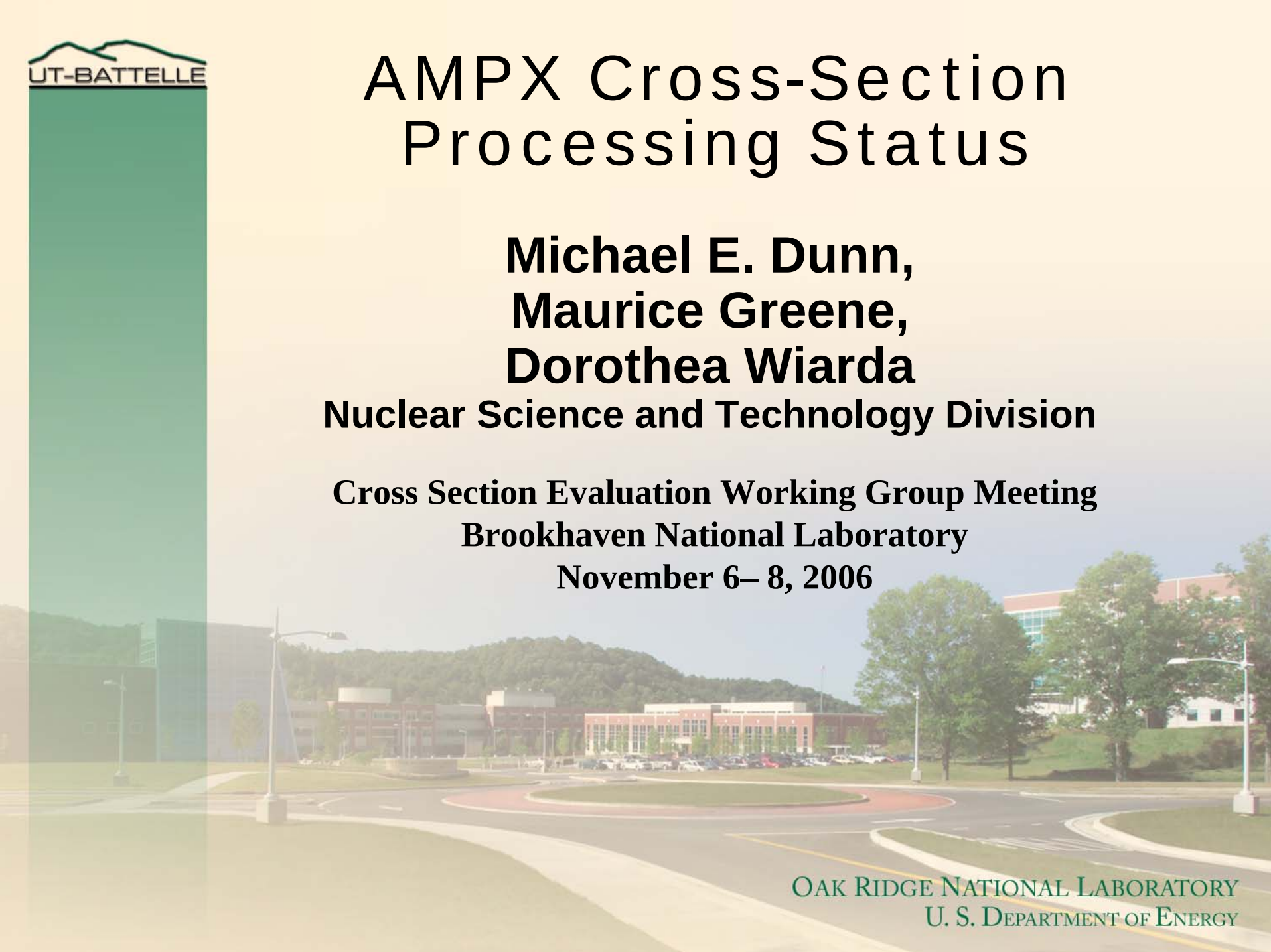
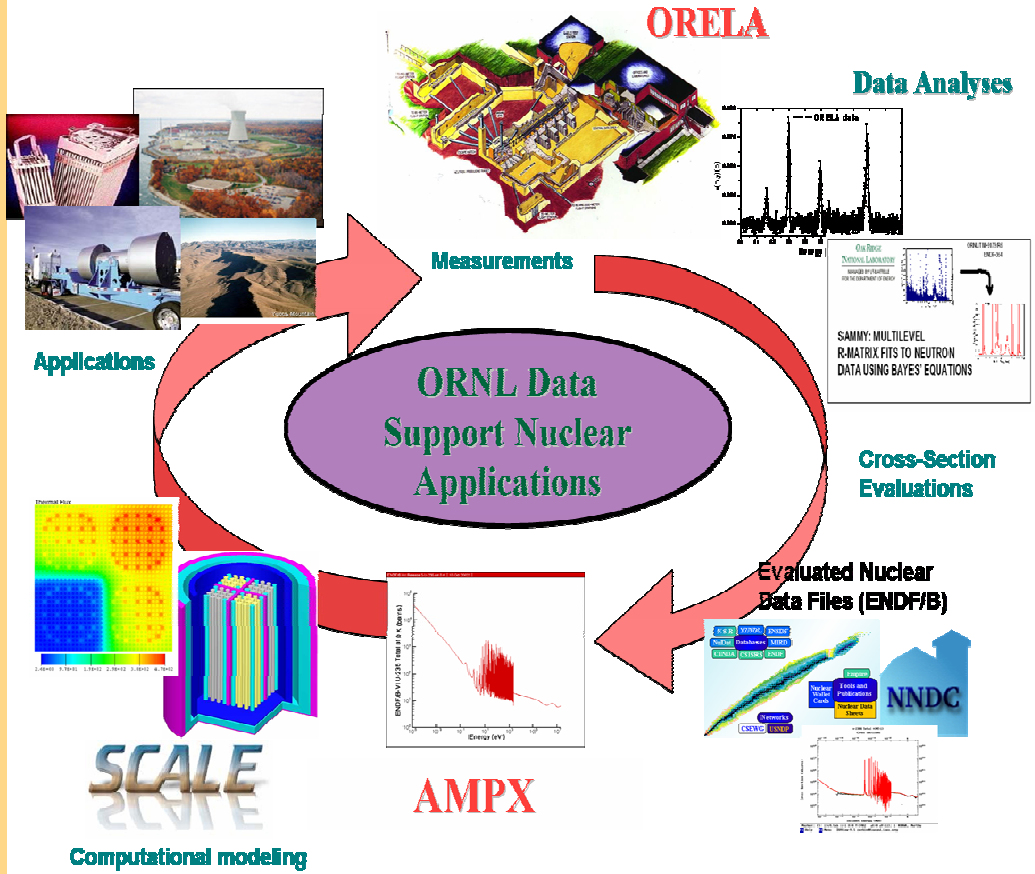


OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

AMPX Nuclear Data for SCALE

- AMPX development and testing driven by needs to support release of SCALE 5.1 in CY2006
  - **S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuation
  - Emphasis on established and well tested nuclear data libraries—pre ENDF/B-VII
- AMPX status
  - Updated numerous AMPX modules to address problems encountered in production and testing of SCALE ENDF/B-VI multigroup and continuous-energy CENTRM libraries.
    - Incorporated adaptive kinematics meshing scheme and included partial fission reaction treatment in chi matrix
    - **Frozen version of AMPX used to produce final SCALE 5.1 libraries**
    - Testing with over 500 benchmark problems—good performance with SCALE 5.1 and ENDF/B-VI libraries



Library Generation & Testing for SCALE

ENDF/B-VI: 238-group and CE CENTRM

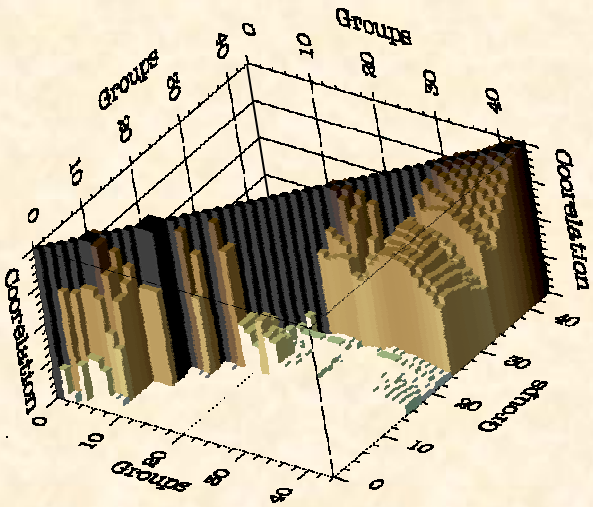
Nuclear Criticality Benchmarks	Total Number of Cases	Number of ICSBEP Cases
Low Enriched Uranium (LEU)	89	33
Intermediate Enriched Uranium (IEU)	21	21
High Enriched Uranium (HEU)	153	149
Mixed Oxide (MOX)	49	32
Pu	101	101
^{233}U	59	59
OECD Benchmark 20: Fuel Dissolver Cases	30	0
Total	502	395

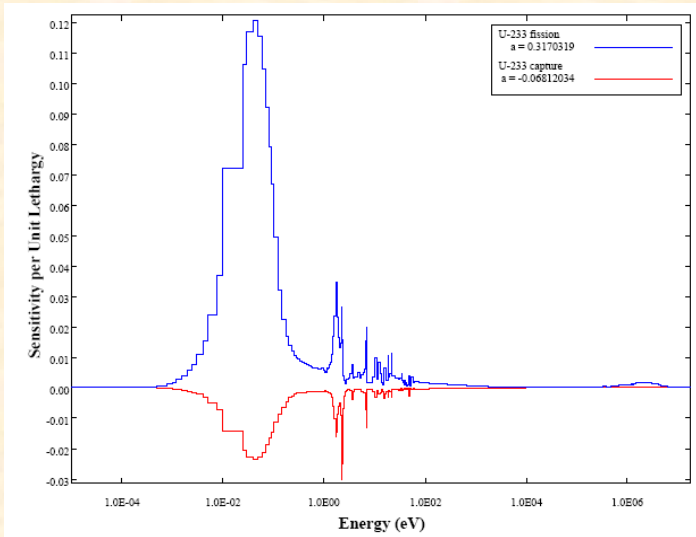
AMPX Nuclear Data for SCALE

- AMPX status (continued)
  - Processed ENDF/B-VII Beta 2 and generated prototypic CE and 238-group libraries
    - Need to add QA identifiers to link MG and CE CENTRM data to support coupled MG and CE radiation transport calculations
    - Need to perform benchmark testing
  - Continuous Energy KENO (**CE-KENO**) 3D Monte Carlo radiation transport software
    - Processed ENDF/B-VI evaluations and generated continuous energy library for all ENDF/B-VI nuclides
    - Testing of CE-KENO software and data with 300+ benchmark problems
    - Training course provided to NRC staff in September—pre-release CE-KENO and library provided to NRC
  - **Finalized and released standalone PUFF-IV code package**
    - **Available from RSICC as Code Package P00534**
    - D. Wiarda and M. E. Dunn ORNL/TM-2006/147
    - Full paper published at PHYSOR 2006 meeting
    - Paper to be published at November ANS Meeting (next week)
    - PUFF will be included as part of AMPX package

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

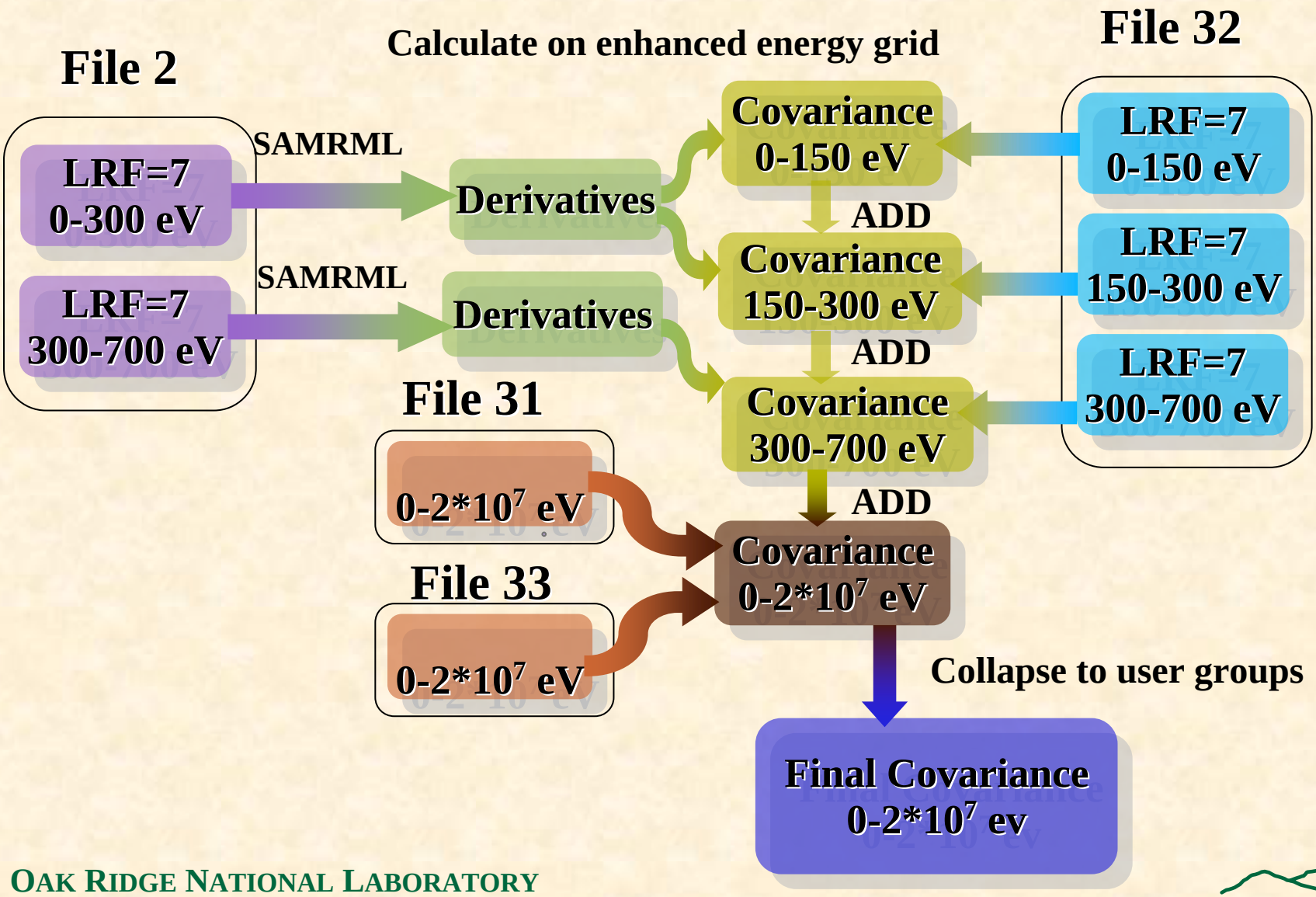
PUFF-IV Module Development for AMPX

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

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.

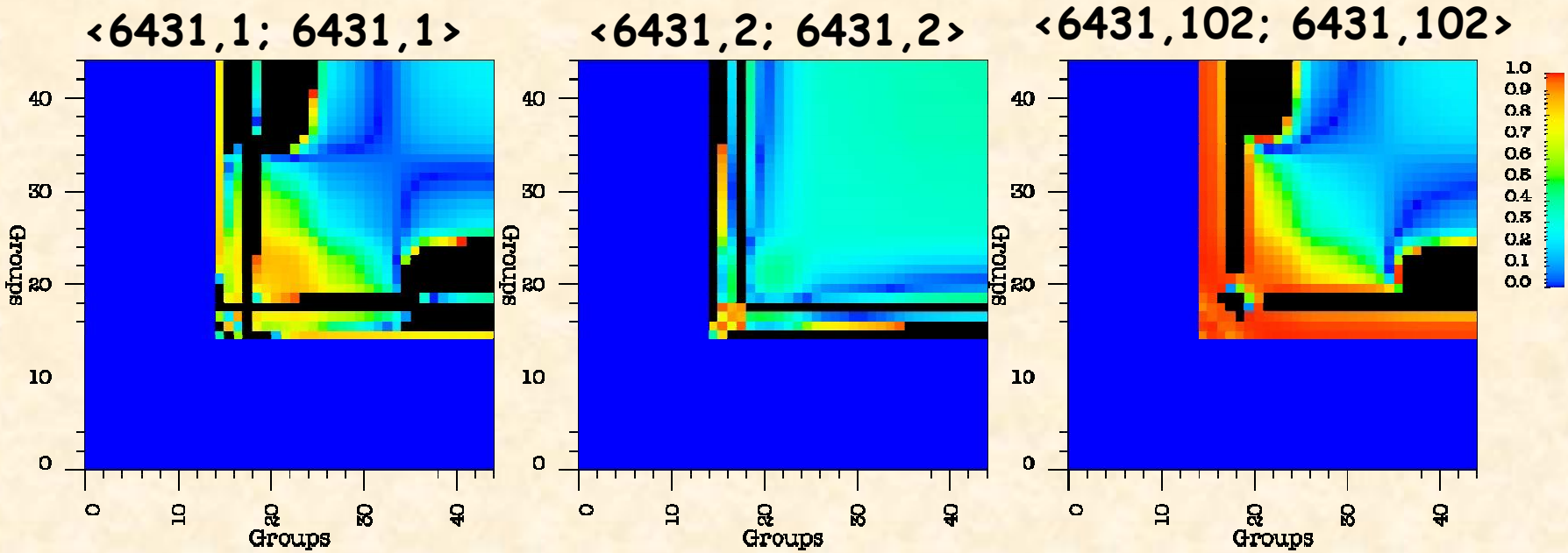
- Added in Beta 3
  ^{10}B std., ^{89}Y, ^{99}Tc, ^{191}Ir, ^{193}Ir

- 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

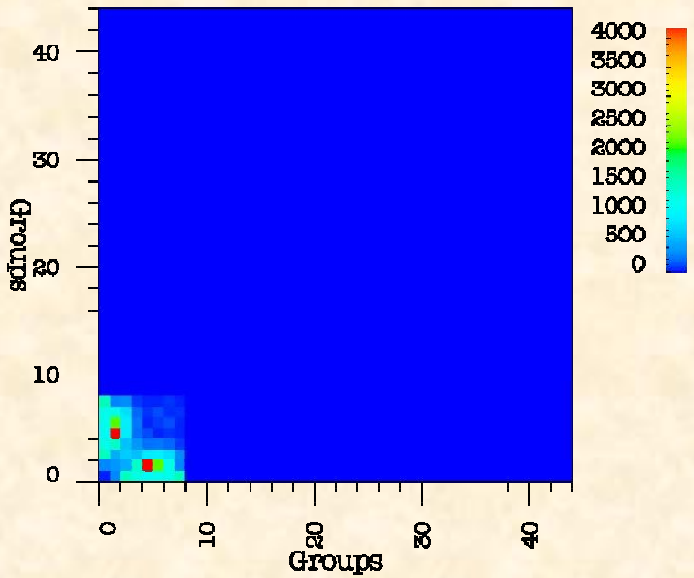
Relative difference >1: black. Largest difference: 180



^{232}Th, MAT=9040

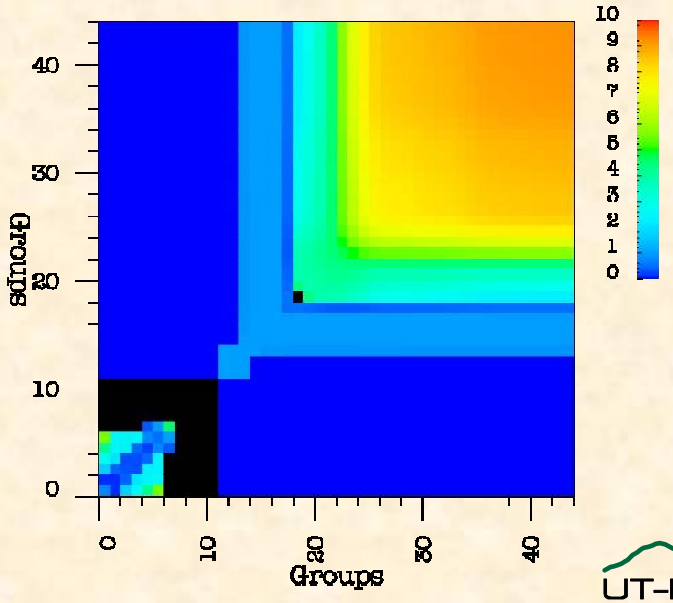
- Changes in resonance parameter covariances are due to changes in uncertainty in thermal values.
- References to ENDV-V numbers have been deleted
- Many cross reaction value covariances matrices are added in File 33
- All high energy covariances data in File 33 are different between Beta 2 and Beta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

<9040,854; 9040,854>



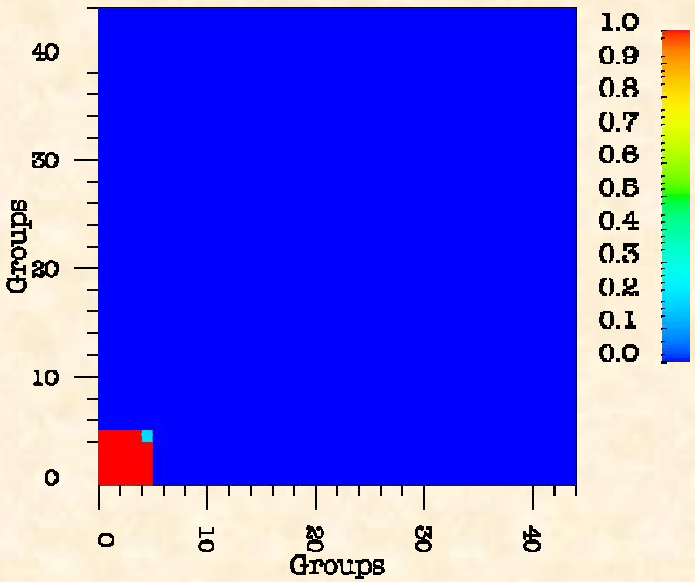
Relative difference >1: black.
Largest difference: 1200

<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.



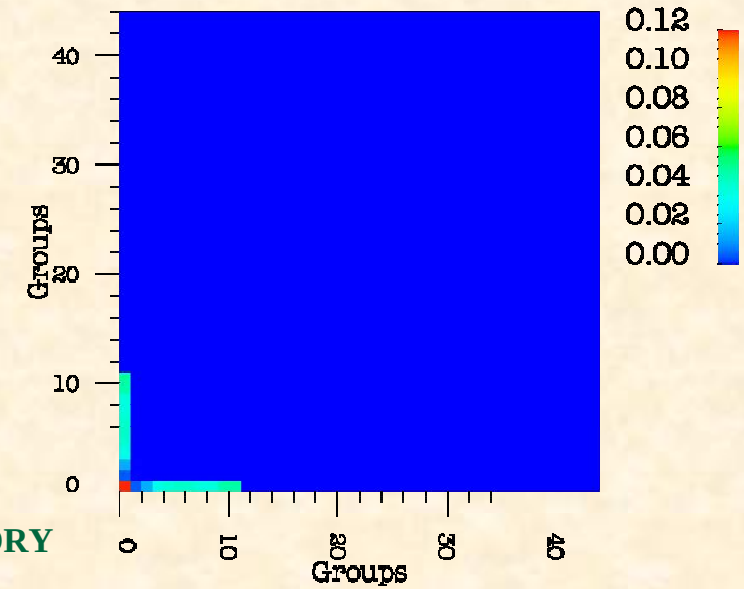
^{6}Li, MAT=325, standard file

- 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

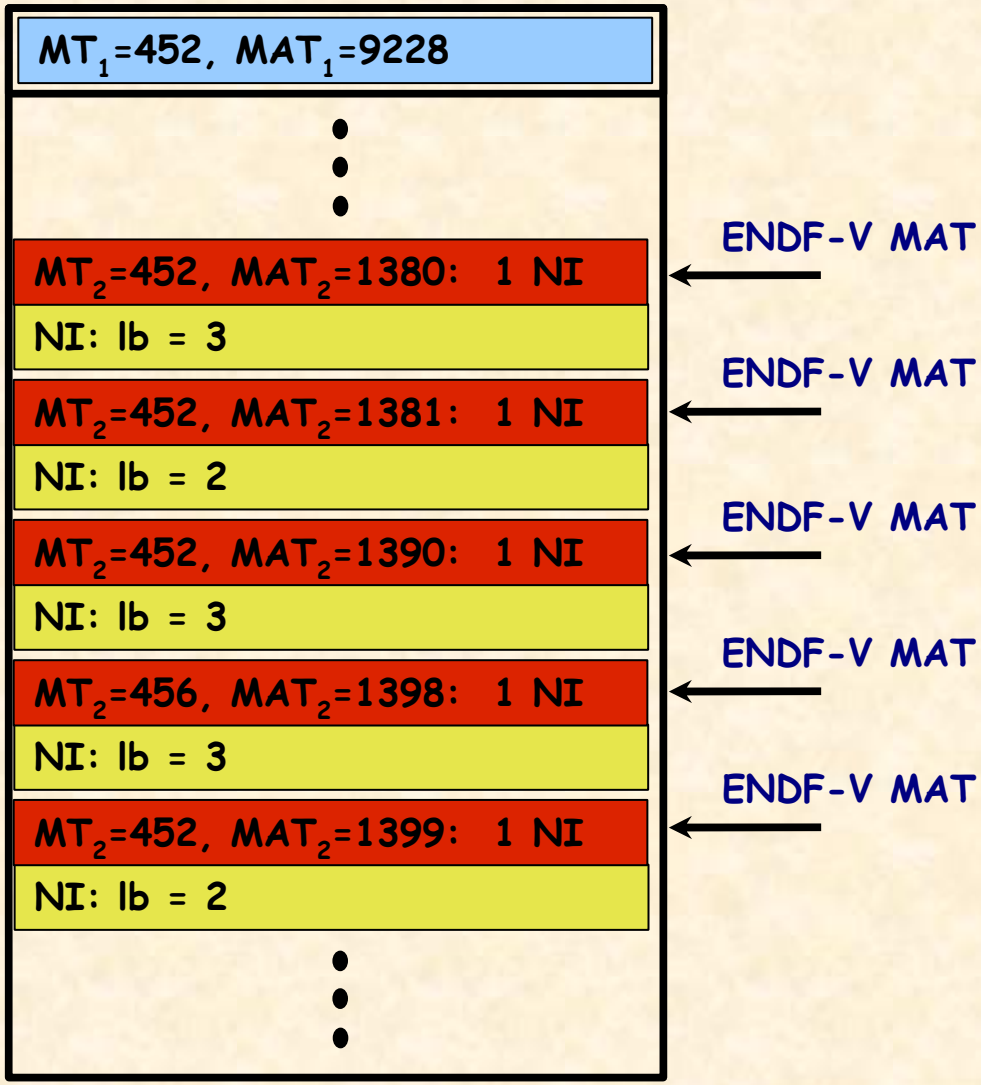
- Components for lumped reaction 851 have been added
- Many more covariances matrices are added in File 33. Among them <328,4; 328,851>.
- Explicit covariance matrices that appear in Beta 2 and Beta 3 are unchanged
- Covariance <328,2; 328,2> is affected by the change since it is given as an NC section,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