

Recent Advances with the AMPX Covariance Processing Capabilities in PUFF-IV

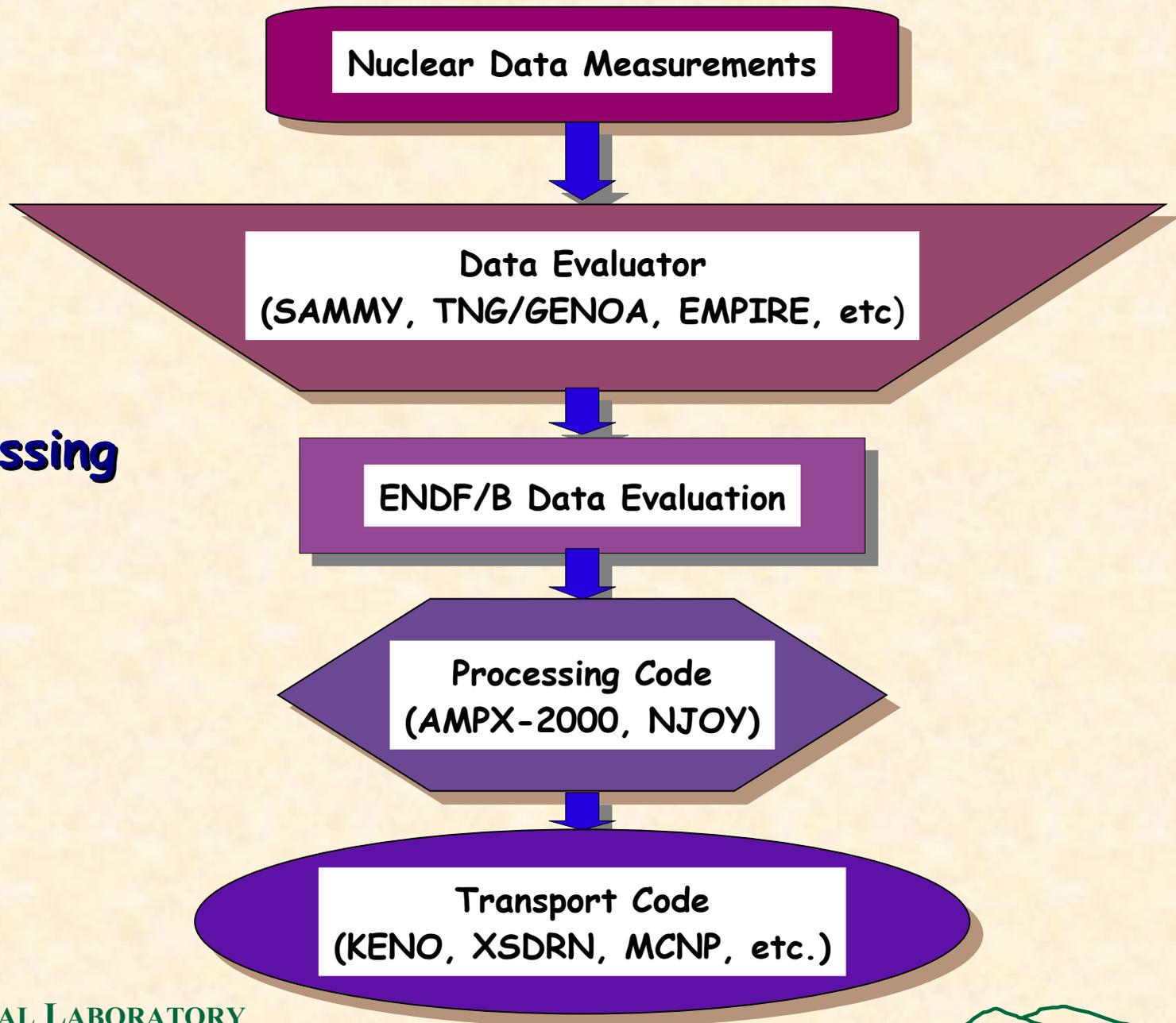
Workshop on Neutron Cross Section Covariances
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BACKGROUND

- PUFF Developed in 1970s to Process ENDF/B-IV Uncertainty Data (FORTRAN-IV; IBM 360/370)
- PUFF-II Developed to Process ENDF Data through Version V (FORTRAN-IV; IBM 3033)
- PUFF-III:
 - ★ Process ENDF Data through Version VI
 - ★ Added to AMPX
- PUFF-IV
 - ★ Rewritten in FORTRAN 90 to allow for a more modular design
 - ★ Add full processing of File 32 resonance parameter covariance data
 - ★ Process ENDF/B-VII uncertainty data

Data Processing Flow



ENDF File Structure

File 1: General information

File 2: Resonance parameters

File 3: Point-wise reaction cross sections

File 31: Data covariance for $\nu(\bar{\nu})$

File 32: Covariance data for resonance parameters

File 33: Data covariance for reaction cross sections

File 2 header: 2 Isotopes

SAMRML
point-wise
derivatives

Isotope 1: Two ranges

LRU=1, LRF=3, [1.0×10^{-5} eV, 100eV]

Resonance parameters

LRU=2, [100eV, 550eV]

Resonance parameters

Combine with
File 32 data
to get
derivatives

SAMRML
point-wise
derivatives

Isotope 2: One range

LRU=1, LRF=7, [1.0×10^{-5} eV, 450eV]

Resonance parameters

LRU

1: resolved
resonance
region

2: unresolved
resonance
region

LRF

1 - 7:
parameter
representation

Group averaged cross section covariance

$$\begin{aligned} \langle \delta x_I^m \delta x_J^l \rangle &= \\ \frac{1}{w_I w_J} \int_I \int_J w(E) w(E') \langle \delta \sigma_m(E) \delta \sigma_l(E') \rangle dE dE' &= \\ \frac{1}{w_I w_J} \sum_{k,n} \langle \delta P_k \delta P_n \rangle \left(\int_I w(E) \frac{\partial \sigma_m(E)}{\partial P_k} dE \right) \left(\int_J w(E') \frac{\partial \sigma_l(E')}{\partial P_n} dE' \right) \end{aligned}$$

Define

$$D_{Ik}^m = \frac{1}{w_I} \int_I w(E) \frac{\partial \sigma_m(E)}{\partial P_k} dE$$

Group averaged:

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

Isotopes and Ranges can be calculated separately and added together as there are no correlations between them

Group averaged cross section covariance

Group averaged:

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

with

$$D_{Ik}^m = \frac{1}{w_I} \int_I w(E) \frac{\partial \sigma_m(E)}{\partial P_k} dE$$

File 32

samrml

Calculate integral with Fourth-Order Runge-Kutta with adaptive step size

Need to calculate the following sum:

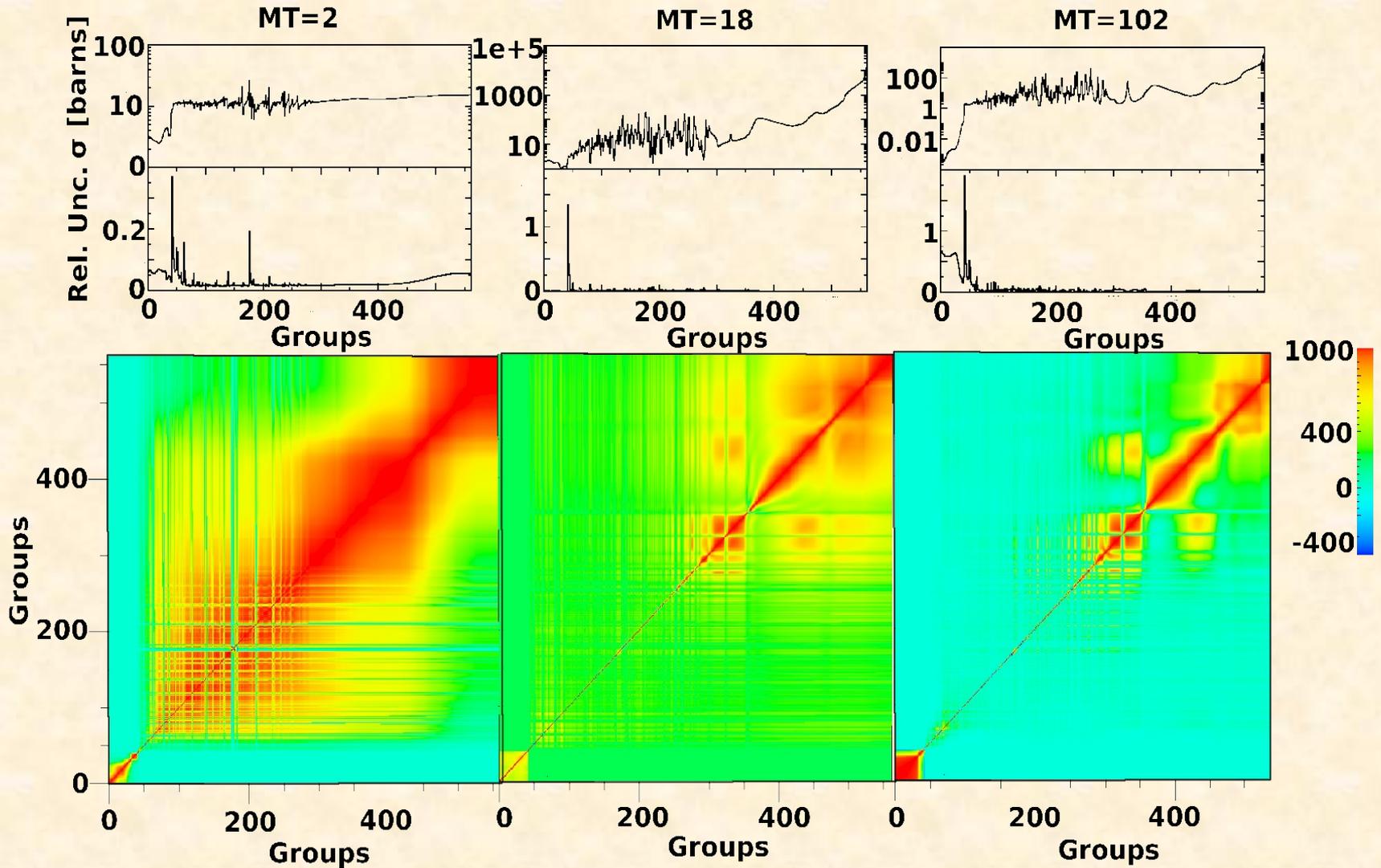
$$\langle \delta x_I^m \delta x_J^l \rangle = \sum_{kn} D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l$$

- For each matrix element sum is over all resonance parameters
- Matrix needs to be calculated for all reactions and cross reactions
- This is the most time consuming task and it scales with the number of resonance parameters and user energy groups.

To speed up calculations

- Set "small" values of D_{Ik}^m to 0 to eliminate terms
- If available use BLAS methods for matrix multiplication

^{235}U on a 562 group structure



Conversion of File 32 to File 33

- File 32 contains Resonance covariance information
- Depending on the number of resonances, File 32 can be big
- ^{235}U has 3193 resonance with 5 parameters each
- The ENDF file is ~2Gb big

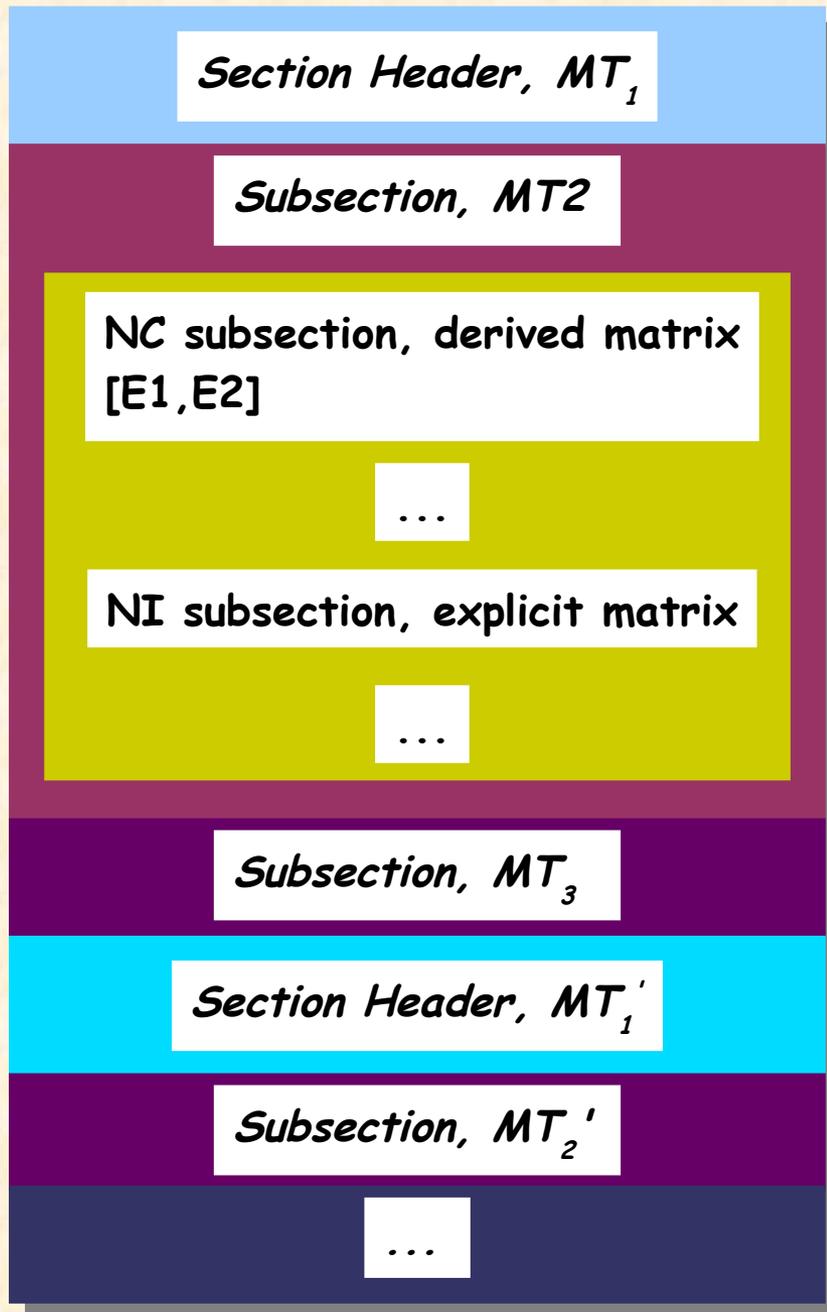
- Can File 32 be transformed to File 33 format and thus reduce the file size requirement?

File 31 or File 33

$\langle MT_1, MT_2 \rangle$

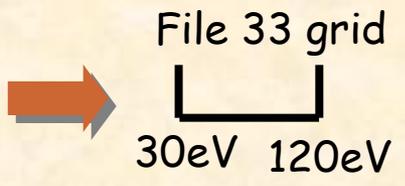
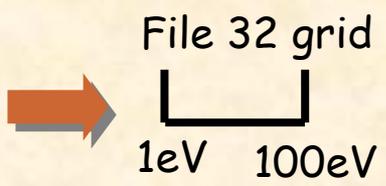
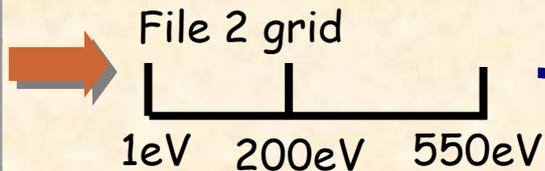
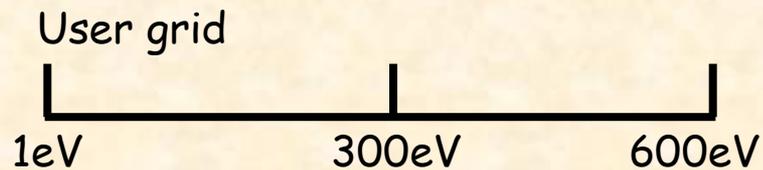
$\langle MT_1, MT_3 \rangle$

$\langle MT_1', MT_2' \rangle$

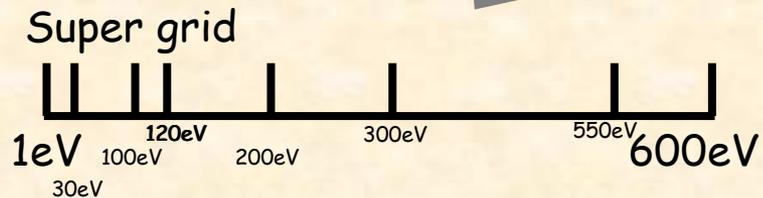


Strategy for Conversion

- Write File 32 covariance matrix information into a COVERX formatted file
- Convert the COVERX file to File 33 format
- Merge with existing File 33 file containing the high energy covariance information.



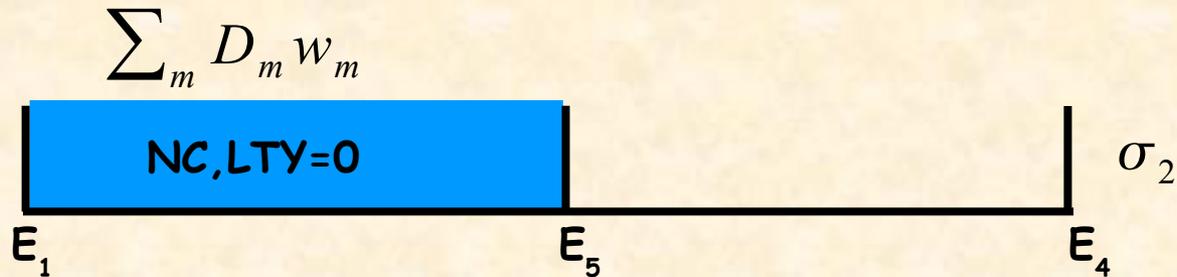
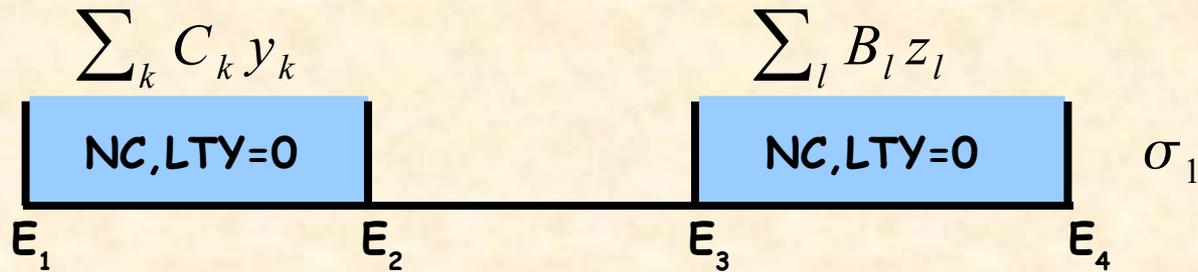
Combine with
User grid
to form
Super grid



Strategy for Conversion

- Need File 32 covariances on super grid
Added an option to PUFF that allows that
- Assume that a constant flux generates suitable histogram for point-wise covariance information
- Need to pick suitable energy grid for conversion
- Grid depends on nuclide
- Speed up due to BLAS allows to experiment with suitable grid

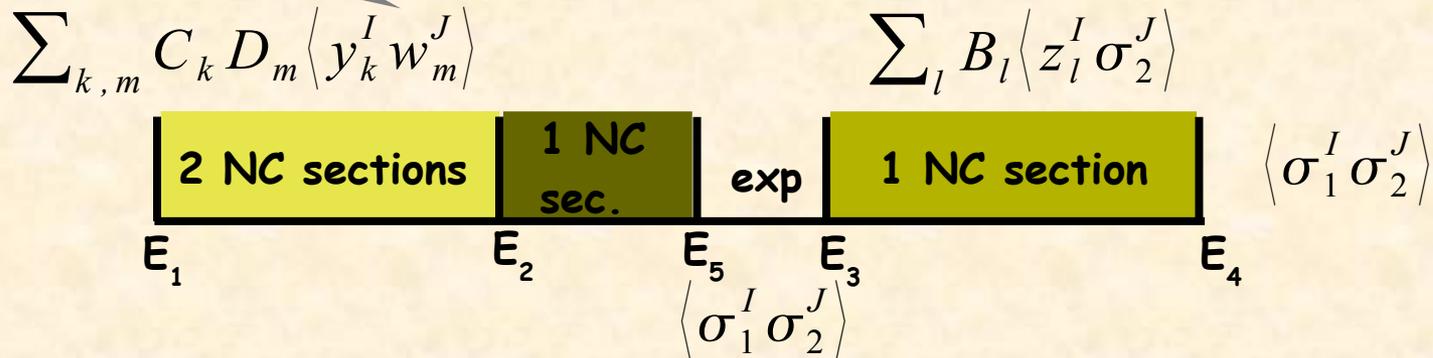
NC Section with LTY=0



Explicit NI sections



Super grid contains all NC boundaries



Merge COVERX covariances into existing File 33

- Convert all matrices to lb=5 format:
Upper triangular relative covariance matrix
- If no LTY=0 sections exist, simply add to File 33 as new NI section, i.e. explicit covariance matrix
- If LTY=0 section exist:
 - ★ Change lower energy boundary of section and import all matrices from the COVERX file
 - ★ Leave LTY=0 section and do not import any matrix defined by this section.

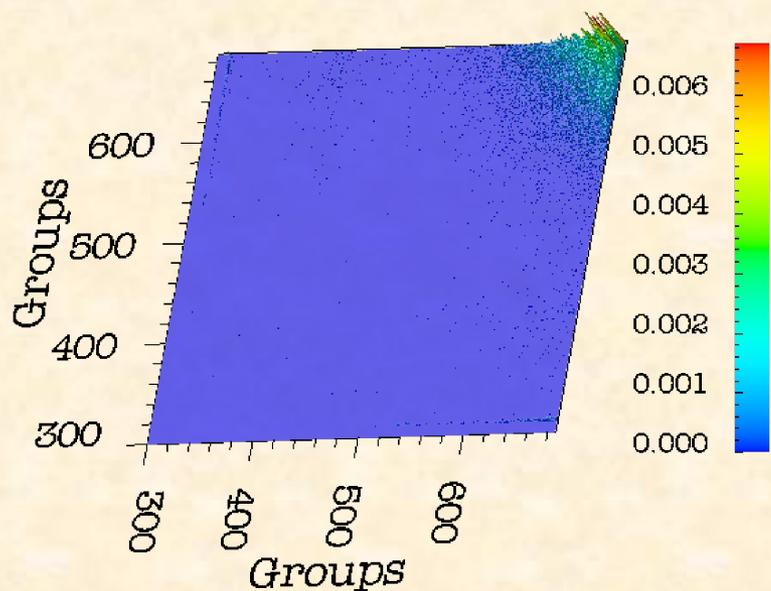
The above is done with program COVCONV
Both options for LTY=0 treatment are available.
We choose the first one

Simulate $l_{ty}=0$ section using COVERX file for ^{235}U

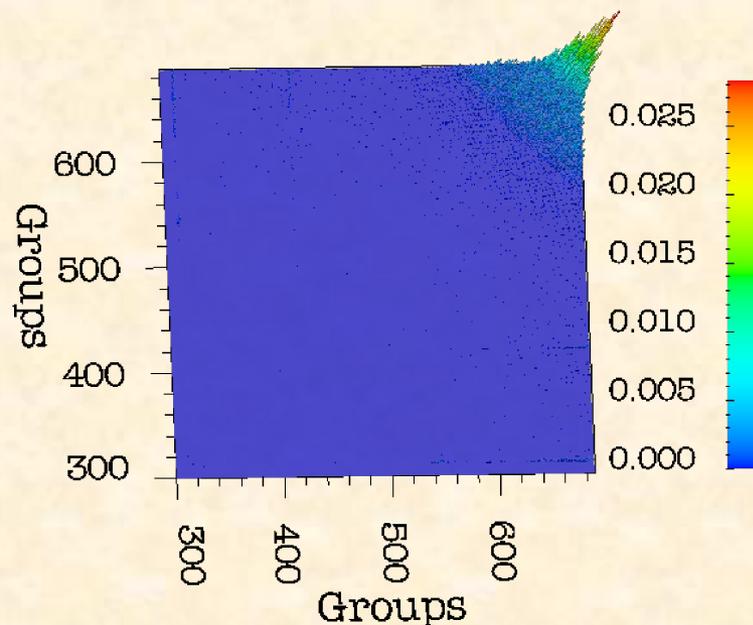
$$\sigma_{elastic} = \sigma_{total} - \sigma_{capture} - \sigma_{fission}$$

Relative difference between absolute uncertainty
from above formula or directly from file

Use single precision binary COVERX

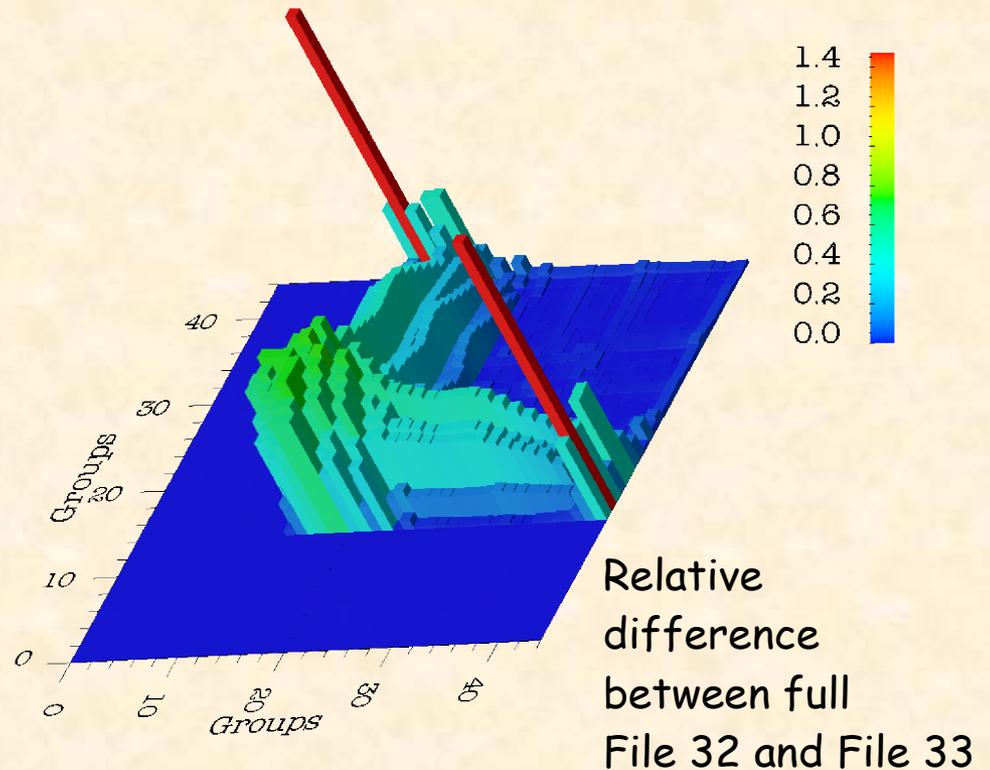
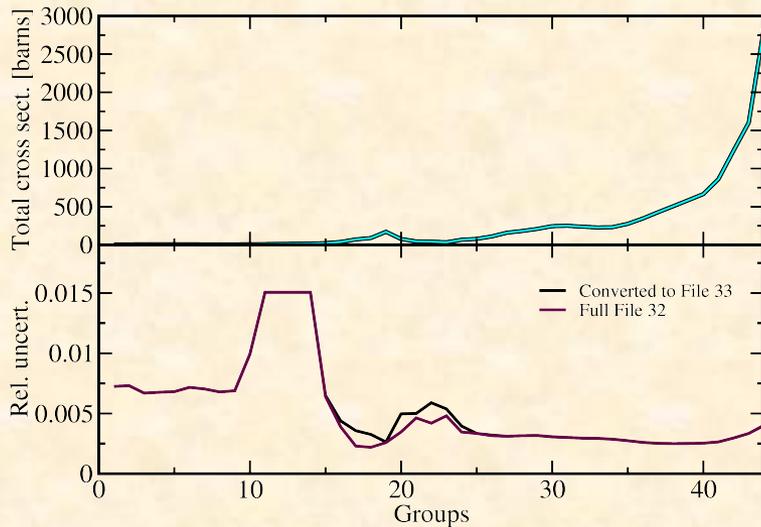


Use endf a11 format



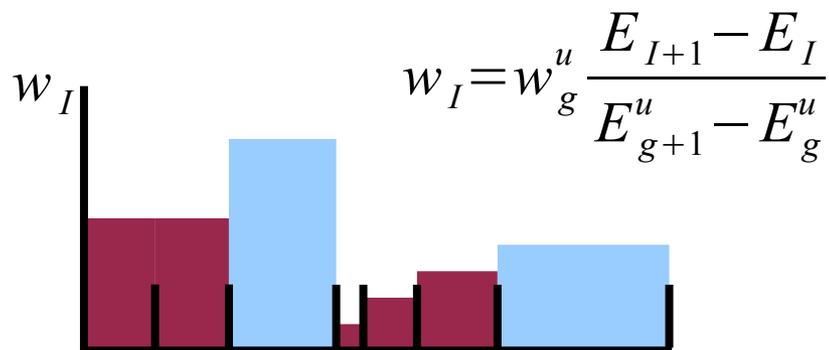
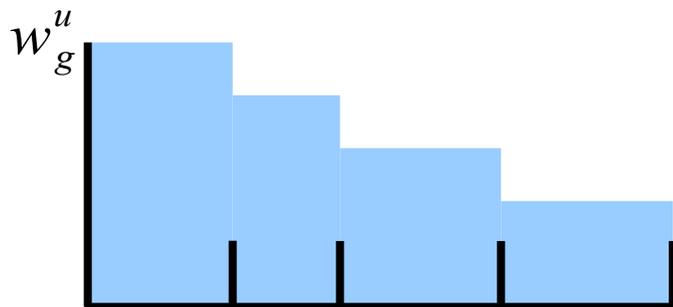
Differences between full File 32 and File 32 -> File 33

Total cross section ^{235}U on
44 group using 44 group
AMPX library



If the same AMPX library (i.e. with 562 groups) is used to create File 33 almost no differences are found

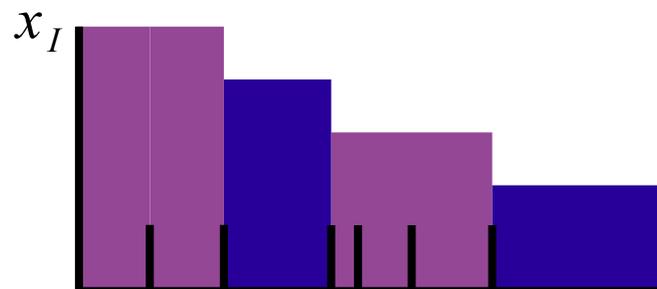
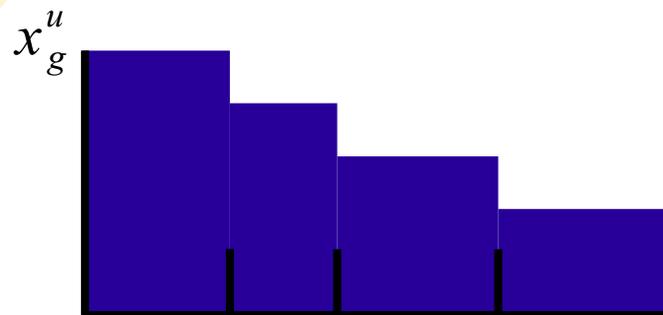
Weight function on super grid



$$w_I = w_g^u \frac{E_{I+1} - E_I}{E_{g+1}^u - E_g^u}$$

$$x_g^u = \frac{1}{w_g^u} \int_{E_g^u}^{E_{g+1}^u} w(E) \sigma(E) dE$$

Cross section on super grid



$$x_I = \frac{1}{w_I} w_g^u x_g^u \frac{E_{I+1} - E_I}{E_{g+1}^u - E_g^u}$$

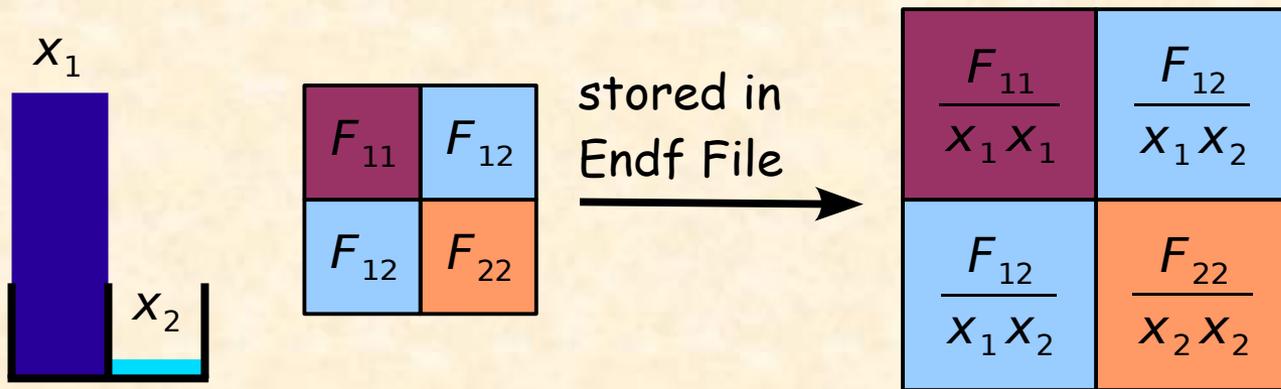
Calculate group cross section data

$$x_I = \frac{1}{w_I} \int_{E_I}^{E_{I+1}} w(E) \sigma(E) dE$$

$$w_I = \int_{E_I}^{E_{I+1}} w(E) dE$$

Calculate group covariance data

$$\langle \delta x_I \delta x_J \rangle = \frac{1}{w_I w_J} \int_{E_I}^{E_{I+1}} \int_{E_J}^{E_{J+1}} w(E) w(E') \langle \delta \sigma(E) \delta \sigma(E') \rangle dE dE'$$



User wants covariance on collapsed group

\bar{x}



$$w_1 = w_2 = 0.5$$

Expected covariance element

$$0.25 F_{11} + 0.5 F_{12} + 0.25 F_{22}$$

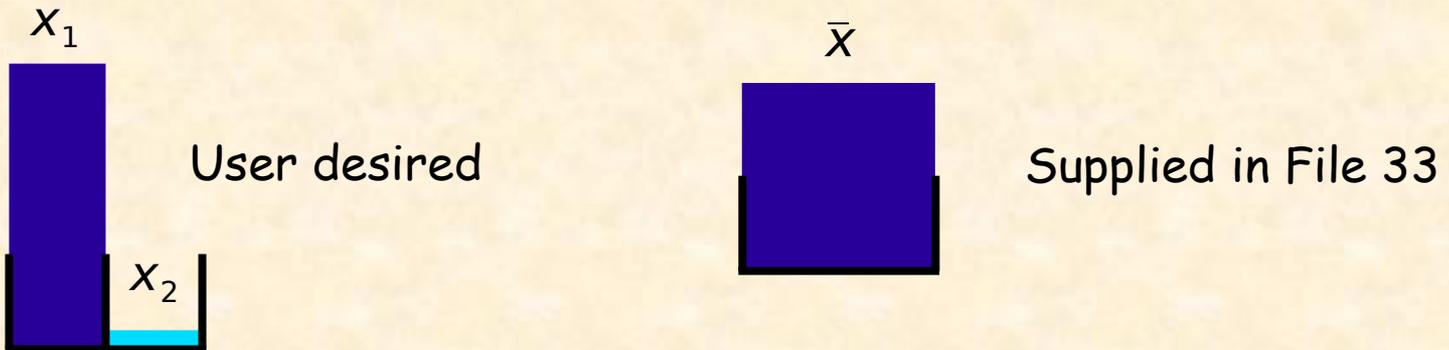
Calculated covariance element

$$0.25 F_{11} \frac{(\bar{x})^2}{(x_1)^2} + 0.5 F_{12} \frac{(\bar{x})^2}{x_1 x_2} + 0.25 F_{22} \frac{(\bar{x})^2}{(x_2)^2}$$

Of course the situation is not that bad

Great care went into selecting a suitable group structure for File 32 -> File 33 conversion

Thus there will not be any conversion:

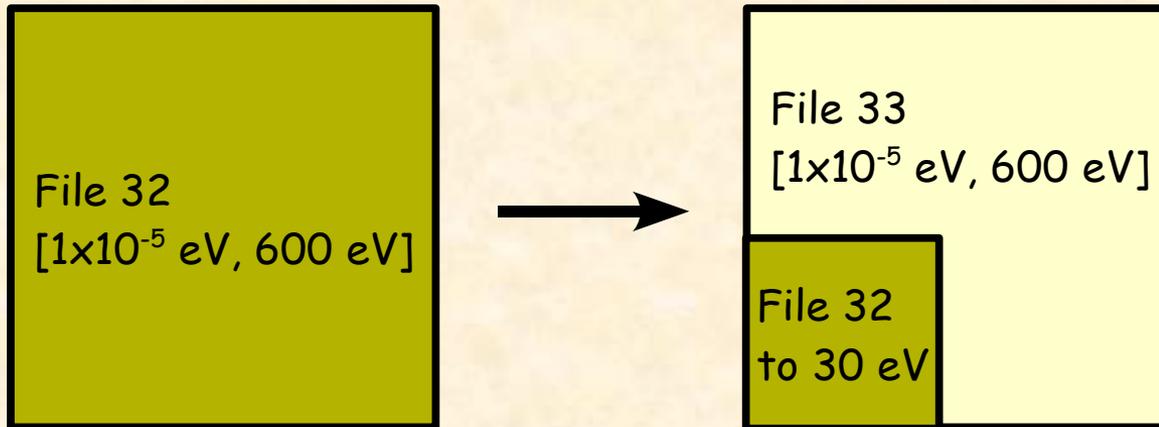


If the user selected exactly the group structure given in File 33, we good agreement

Full File 32 covariance file is available from ORNL

SCALE covariance libraries use full File 32

Hybrid method



The added File 33 portion still extends over the whole resolved resonance range, but has zeros where the reduced File 32 is used. This allows to capture correlation between the two energy regions.

Question: How do create the reduced File 32 and File 33
Method is not implemented but was tested on ^{233}U using a modified PUFF-IV version. Energy boundaries will depend on nuclide.

File 2

File 32

File 31 + File 33

LRU=1, LRF=3
[$1 \times 10^{-5} \text{eV}$, 100eV]

LRU=2
[100eV, 550eV]

LRU=1, LRF=3
[$1 \times 10^{-5} \text{eV}$, 100eV]

LRU=2
[100eV, 550eV]

Covariances
from NI and NC
[$1 \times 10^{-5} \text{eV}$, $2 \times 10^7 \text{eV}$]

Covariance (Super grid)
[$1 \times 10^{-5} \text{eV}$, 100eV]

Covariance (Super grid)
[100eV, 550eV]

Covariance (Super grid)
[$1 \times 10^{-5} \text{eV}$, $2 \times 10^7 \text{eV}$]

Collapse

Combine

Covariance (Super grid)
[$1 \times 10^{-5} \text{eV}$, 550eV]

Covariance (User grid)
[$1 \times 10^{-5} \text{eV}$, $2 \times 10^7 \text{eV}$]

Construct File 32 for hybrid method

- Restrict File 32 range to 30 eV
- Include resonance and corresponding covariance information for all resonance with resonance energy below 100 eV

Define

$$D_{Ik}^m = \frac{1}{w_I} \int_I w(E) \frac{\partial \sigma_m(E)}{\partial P_k} dE$$

Group averaged:

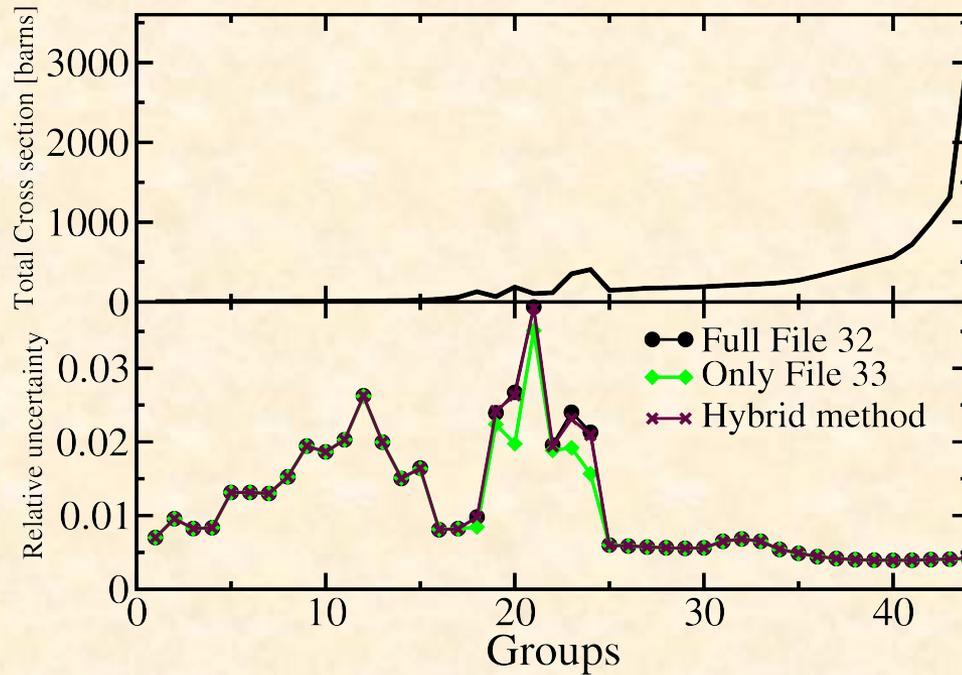
$$\langle \delta x_I^m \delta x_J^l \rangle = \sum_{kn} D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l$$

Construct File 33 for hybrid method

- Calculate reference File 33 from full File 32.
Use optimized energy grid
- Calculate truncated File 33 from truncated File 32
Use optimized energy grid
- Calculate new File 33 as:
reference File 33 - truncated File 33
- This ensures that correlations between the two energy ranges
are accounted for

Merge new File 33 with existing high energy File 33 data
Add File 32 to make a full ENDF file

^{233}U Comparison first results



SUMMARY

- PUFF-IV processes ENDF uncertainty data and generates multigroup covariance and correlation matrices for a user-specified energy structure
- Processing of File 32 covariance was sped up via the use of BLAS routines
- In order to minimize ENDF files, a program (COVCONV) was developed to convert File 32 into File 33
- A possible hybrid method was discussed to allow the use of File 32 in the lower energy region ($\sim 30\text{eV}$) and File 33 above.

How to obtain code

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.**

**We are expecting to release a new version
which includes the enhancements discussed**