ORNL Cross-Section Processing Status

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Outline

- **AMPX Nuclear Data Support for SCALE 5 Radiation Transport Package**
- **Generation & Testing of Continuous-Energy & Multigroup Cross-Section Libraries**
- **Covariance Data Processing Improvements**

AMPX Nuclear Data for SCALE

- **SCALE 5.0 released summer 2004**
  - CE CENTRM libraries to "match" 238-group ENDF/B-V library
  - MG ENDF/B-V covariance data for TSUNAMI
  - Expanded and Improved ORIGEN data based on ENDF/B-VI, EAF-99, FENDL-2.0, ENSDF libraries
- **SCALE 5.1**
  - CENTRM resonance processing updates
    - Improved memory management and efficiency
    - Improved thermal calculations with bound scattering kernels
    - Updates to address lattice effects in non-uniform lattices
    - Developed new SCALE sequence to address double-heterogeneity effects in resonance self-shielding—pebble bed reactors
    - Developed capability to compute Dancoff factors in general geometry using 3-D Monte Carlo—release after SCALE 5.1
  - CE CENTRM and 238-group ENDF/B-VI.7 libraries
    - CE cross-section data as a function of temperature $\sigma(E,T)$
    - Collision kinematics kernels for thermal moderators
  - Release CE and MG ENDF/B-VI.7 Libraries with SCALE 5.1
- **Beyond SCALE 5.1**
  - Fine-group (400+ neutron groups) ENDF/B-VI Library
  - Coupled neutron-gamma libraries
  - CE KENO Monte Carlo Libraries
  - CE and MG ENDF/B-VII Libraries
  - Expanded covariance data information for TSUNAMI

Covariance Data Processing Improvements

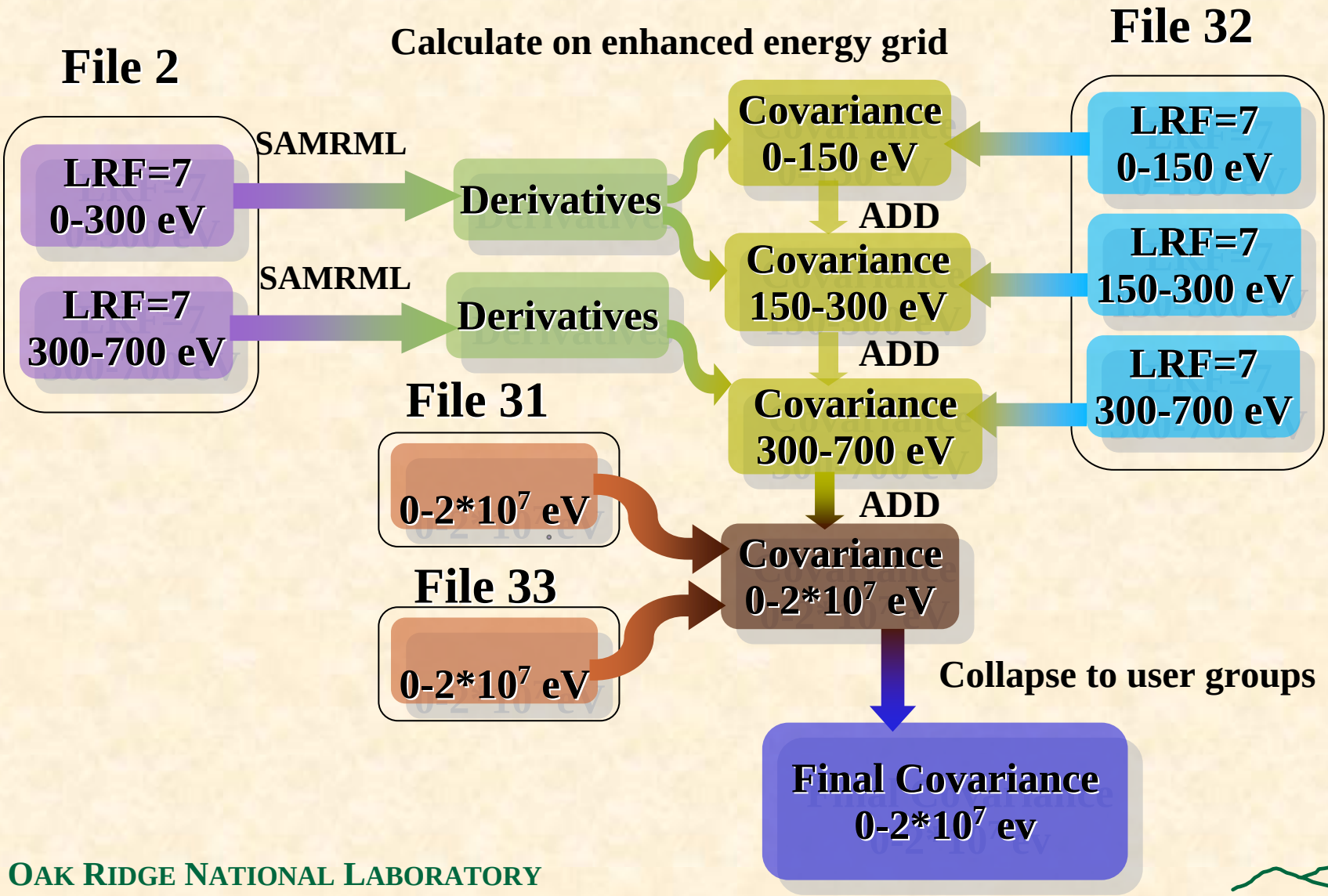
PUFF-IV Module Development for AMPX

- Complete rewrite of PUFF-III code in F90.
- Object oriented design as far as possible in F90.
- Results are the same as in PUFF-III within rounding errors
- Automatic test cases comparing PUFF-III results and PUFF-IV results

File 32 processing

- Derivatives are calculated from File 2 using SAMRML
- Group averages of covariances are calculated using the above derivatives
- Only resolved 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 covarianace 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

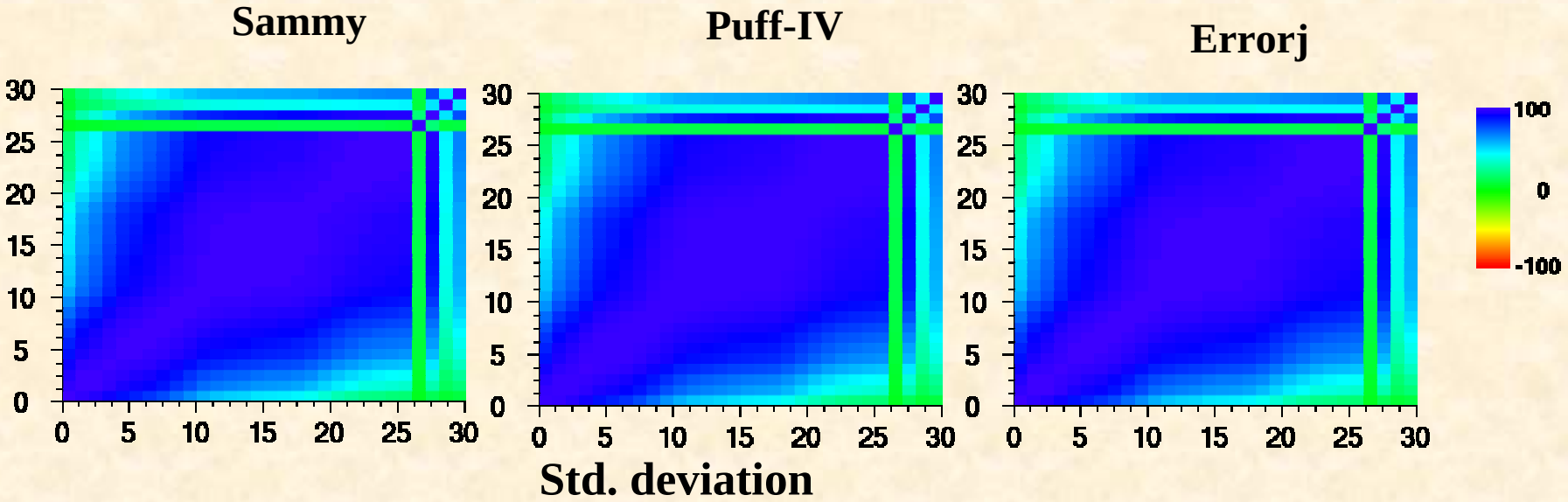
$$\langle \delta x_I^m \delta x_J^l \rangle = \sum D_{Ik}^m \langle \delta P_k \delta P_n \rangle D_{Jn}^l$$

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



Largest absolute difference:

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

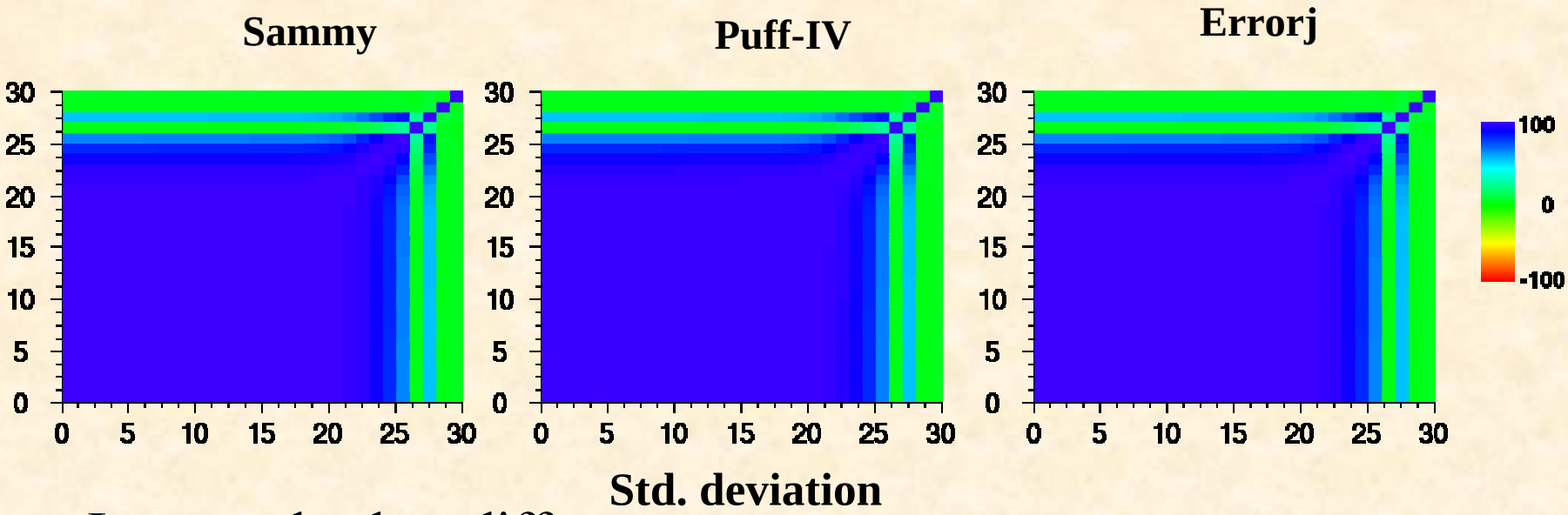
Errorj -Puff-IV: $5.22*10^{-6}$

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

^{158}Gd resolved region only: Capture cross section - flat flux

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

Correlation matrices



Largest absolute difference:

Errorj -Sammy: $1.53*10^{-5}$

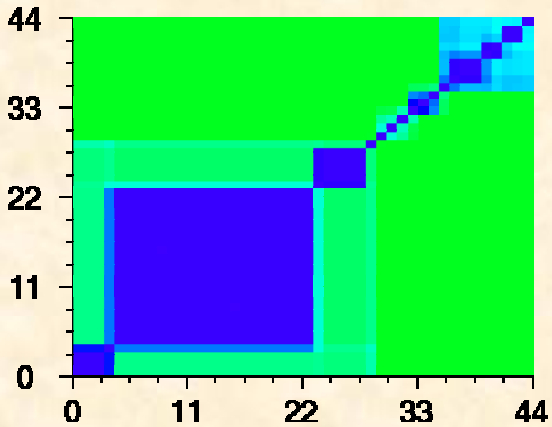
Errorj -Puff-IV: $2.31*10^{-5}$

Sammy - Puff-IV: $9.0*10^{-6}$

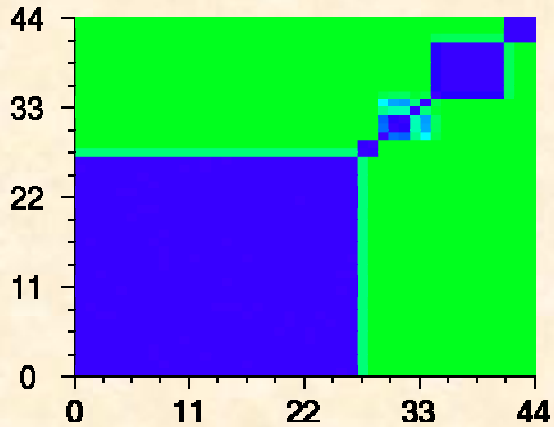
^{23}Na: File 33 and File 32 processing – flat flux

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

Total cross section



Capture cross section



PUFF-IV Future Development Tasks

- More tests with new ENDF/B-VII cases containing lrf=7 covariance evaluations.
- Complete documentation
- Unresolved resonance region—derivatives could be calculated numerically using existing AMPX routines that calculate cross section data in the unresolved region.