

# AMPX Cross-Section Processing Status

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## AMPX Nuclear Data for SCALE

- AMPX development and testing driven by needs to support release of SCALE 6 in CY2008
  - Standardized Computer Analyses for Licensing Evaluation
  - New data libraries based on ENDF/B-VI.8 and ENDF/B-VII.0

#### AMPX status

- Updated numerous AMPX modules to address problems encountered in production and testing of SCALE ENDF/B-VI and ENDF/B-VII multigroup and continuous-energy libraries.
  - Incorporated adaptive meshing scheme for Doppler Broadening
  - Testing with over 1300 benchmark problems—good performance with SCALE 6
- PUFF-IV updated to produce new SCALE 6 covariance library
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### AMPX Nuclear Data for SCALE 6

- ENDF/B-VI.8 238 neutron group general purpose library
- ENDF/B-VII.0 238 neutron group general purpose library
- ENDF/B-VI.8 200 neutron/47 gamma coupled shielding library
- ENDF/B-VII.0 200 neutron/47 gamma coupled shielding library
- ENDF/B-VII.0 27 neutron/19 gamma coupled library primarily to perform adjoint discrete ordinance calculations.
- ENDF/B-V, ENDF/B-VI.8 and ENDF/B-VII.0 continuous energy libraries
- Comprehensive Covariance library for use with all libraries.
  Low-fidelity data are used if no other data are available.

#### Library features

- Full range Bondarenko factors for multi-group libraries
- CE Data for Resonance Region self shielding

Data format for continuous energy CENTRM data to use the same library for multi-group self-shielding calculations and for continuous energy KENO calculation.



### PUFF-IV Sources of Covariance Data in SCALE 6

Source	Materials						
ENDF/B-VII.0	Li <sup>7</sup> Ti <sup>48</sup> Y <sup>89</sup> , Gd <sup>152-158,160</sup> Th <sup>232</sup> Tc <sup>99</sup> Ir <sup>191,193</sup>						
ENDF/B-VII	U <sup>233,235,238</sup> Pu <sup>239</sup> , Mn <sup>55</sup>						
pre-release							
	Na <sup>23</sup> Al <sup>27</sup> Si <sup>28-29</sup> Sc <sup>45</sup> Cr <sup>50,52-54</sup> Fe <sup>54,56-58</sup>						
ENDF/B-VI	Ni <sup>58,60-62,64</sup> Cu <sup>63,65</sup> Nb <sup>93</sup> In <sup>(nat)</sup> Au <sup>197</sup>						
	Pb <sup>206-208</sup> Bi <sup>209</sup> Am <sup>241</sup> pu <sup>242</sup>						
JENDL	Pu <sup>240-241</sup> - nu-bar for U <sup>235</sup>						
LANL	H <sup>2,3</sup> He <sup>4</sup> Li <sup>6,7</sup> Be <sup>9</sup> B <sup>11</sup> C <sup>(nat)</sup> C <sup>12</sup> N <sup>14-15</sup>						
NCSP Low-Fi Proj.	O <sup>17</sup> F <sup>19</sup>						
NCSP Low-Fi	>200 materials						
Proj.							

OAK RIDGE NATIONAL LABORATORY U. S. DEPARTMENT OF ENERGY SG26 covariances using ORNL low-fidelity below 0.625 eV U<sup>234,236</sup> Np<sup>237</sup> Pu<sup>238</sup>

Am<sup>242, 242m</sup> Cm<sup>242-245</sup>

LANL covariances using ORNL low-fidelity below 5 keV <sup>3</sup>He

LANL covariances below 5 keV use H<sup>1</sup> - JENDL3.3 O<sup>16</sup> - JENDL3.3 B<sup>10</sup> - ENDF/B-V



### Merging of File 33 data

To produce SCALE covariance library using approximate covariance data



Thermal range: use thermal cross sections and uncertainties up to 0.625 eV

Epithermal range: use resonance integral sections and uncertainties 0.625 eV - 5 keV

- Always use thermal cross section data for elastic scattering
- Use thermal cross section data if no resonance integral data are available
- Above 5 keV BNL Low-fidelity data, ENDF/B-VI, ENDF/B-V or JENDL



#### Post processing of Covariance information for SCALE 6

- Any relative uncertainty above 100% is set to 100%
  Correlations are preserved
- For total, elastic, capture and fission: high energy range uncertainties are extended to low energy if low energy uncertainties are not available.

Use functionality in module covcomp to easily analyze and change coverx files

Often for threshold reaction, for example Ni<sup>64</sup> (n, alpha) File 33 gives

- Ib=0 or absolute covariance matrix
- additional section with relative covariance matrices



ni64 (n,alpha)

#### PUFF-IV version 6.1.0 submitted to RSICC

- Various bug fixes concerning calculation of derivatives and group averaging of derivatives
- Improved processing of Irf=7 covariance matrices
- Support for BLAS to decrease computation time in the resolved resonance range
- Support for user defined flux functions
- Module covcomp has additional functionality for comparing and adding coverx formatted files
- Module coverr allows to convert COVERX files to NJOY covariances tapes



0.0

0.0



#### Broaden

Added adaptive temperature dependent energy mesh to better describe resonances and discontinuities. This improves benchmark results for the Big10 benchmark. This also leads to better agreements with NJOY results.



All codes use these broadened data to calculate continuous energy data, multi-group data and Bondarenko factors.



#### Continuous energy libraries

- Continuous energy libraries are used for multi-group shielding calculations as well as continuous energy KENO calculation.
- SCALE 6 format changed to allow use of the same library in both cases, except for scattering kernel
- Converted ENDF/B-V continuous energy data into new format.
- Fixed several AMPX modules to support new format.
- Save various additional reactions for use in KENO
- Doppler broaden and save partial fission reactions for use in KENO
- Moved unresolved resonance calculation into endfLib to ensure consistent results across all AMPX modules.









#### Most AMPX modules have automated test cases

1e-3 # precision to which to compare to ----- AMPX input (please use default units) % endf is replaced by mat 0\$\$ 31 32 e 1\$\$ 1 t 2\$\$ %endf% 11 2 6 e 4\*\* 0.001 e 6\$\$ a3 0 15000 e t ----- test cases: first is mat number, endf file name, tab1 std. file 1825 ar36\_tab1(b) ar36.endf 125 h1\_tab1(b) h1.endf 3000 zn\_tab1(b) zn.endf 4125 nb93\_tab1(b) nb93.endf 1225 mg24\_tab1(b) mg24.endf 1325 al27\_tab1(b) al27.endf 1825 ar36\_tab1(b) ar36.endf 925 f19\_tab1(b) f19.endf 9219 u232\_tab1(b) u232.endf 9225 u234\_tab1(b) u234.endf

>./testcases/testcases

Testing Polident

Checking 1825 with endf file ar36.endf Largest disagreement is 0.000047683716 % Checking 125 with endf file h1.endf Largest disagreement is 0. % Checking 3000 with endf file zn.endf



#### Exsite as future GUI for SCALE and AMPX

Allows to construct and run input files Currently working only for selected SCALE programs





#### Exsite to run and compare benchmark results

File Format Benchmark Scheduler Profile Window Help

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	hst25-04	2	2	heu	0.99950	1.00146	ŏ	crawdad_completion	is finished. completion code
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	hst25-12	21	21	heu	1.00620	1.00724	ŏ	bonami_completion	is finished. completion code
	hst35-08	22	22	heu	0.99894	0.99919	ŏ	worker_time	11:40:49.983 at 10/23/2008.
	hct010-05	23	23	heu	0.99995	0.99669	ŏ	worker_completion	is finished. completion code
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	hct010-18	26	26	heu	1 00486	1.00235	ŏ	pmc time	11:40:47.008 at 10/23/2008.
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can be used for MG and

#### Template engine to produce input files

<Materials> <Material tag="h1" endf="125" <InputData> za="1001" <openFile name="&batch;"/> tape="n-001\_H\_001.endf" <loop restrict="+neutron(yes)"> <openFile name="&case;"/> <Material tag="u238" <writeFile name="&case:"> endf="9237" za="92238" <text>=shell tape="n-092\_U\_238.endf" In -sf &broaden\_file; ft34f001

> end =pickeze -1\$\$ 3000000 0\$\$ 34 35

<!-- pickeze -->

Input for He3

List of endf related information. Retrieved automatically from a directory containing endf files

</Material

Defines sequence Uses a few user defined parameters

Plan to use in Exsite to support "SCALElike" sequences

UT-BATTELLE

#### **Future Development Activities**

- Convert all major modules used for cross section and covariance processing to Fortran 90.
- Convert most modules to do all calculations in double precision.
- Develop the capability to produce a continuous energy gamma library
- Expand Exsite capabilities to serve as GUI for AMPX cross section processing.
- Develop "SCALE-like" sequences
- Prepare libraries for SCALE based on the latest JEFF libraries
- Package and release AMPX by 2010
- Participate in Cross Section Workshop in conjunction with JEFF Meeting (Nov. 18-21, 2008)

