# AMPX Cross-Section Processing Status

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Nuclear Science and Technology Division
Cross Section Evaluation Working Group Meeting
Brookhaven National Laboratory
November 4 – 6, 2008

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AMPX Nuclear Data for SCALE

- 🔴 AMPX development and testing driven by needs to support release of SCALE 6 in CY2008

  - ⭐ **S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuation

  - ⭐ 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 multi-group 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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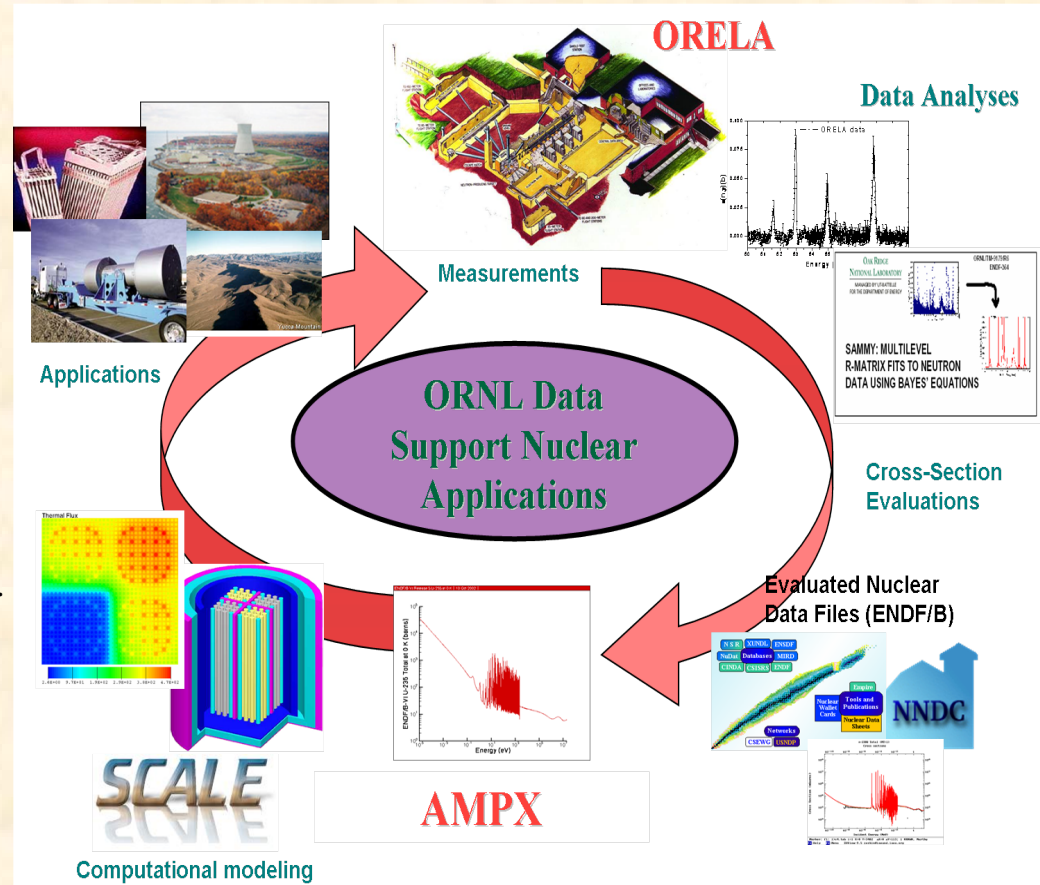
AMPX Nuclear Data for SCALE 6

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

SG26 covariances using ORNL low-fidelity below 0.625 eV

$U^{234,236}$ Np^{237} Pu^{238} $Am^{242, 242m}$ $Cm^{242-245}$

LANL covariances using ORNL low-fidelity below 5 keV
^3He

LANL covariances below 5 keV use
H^1 - JENDL3.3
O^{16} – JENDL3.3
B^{10} - ENDF/B-V

Merging of File 33 data

To produce SCALE covariance library using approximate covariance data

$$cov = \left[\frac{max\left(\Delta_i, \frac{|x_i - X_i|}{2} \right)}{\frac{x_i + X_i}{2}} \right]^2$$

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

Zr^{91}
Capture
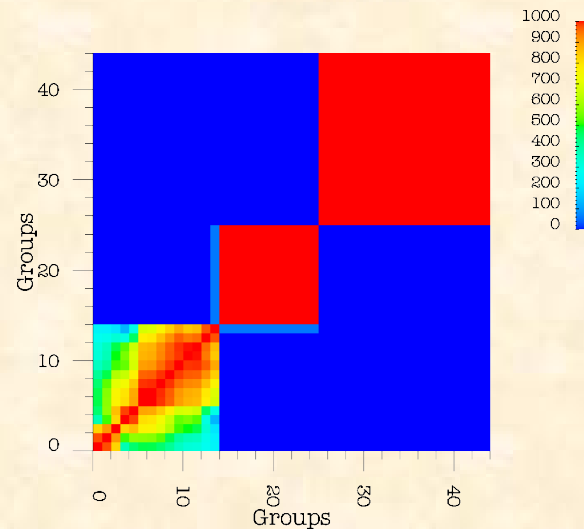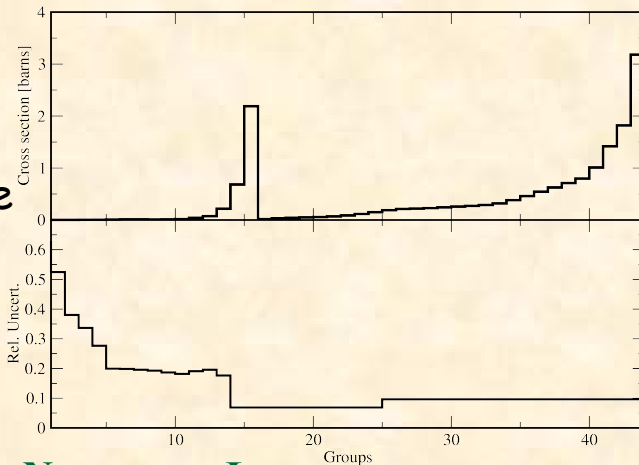
Post processing of Covariance information for SCALE 6

- 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
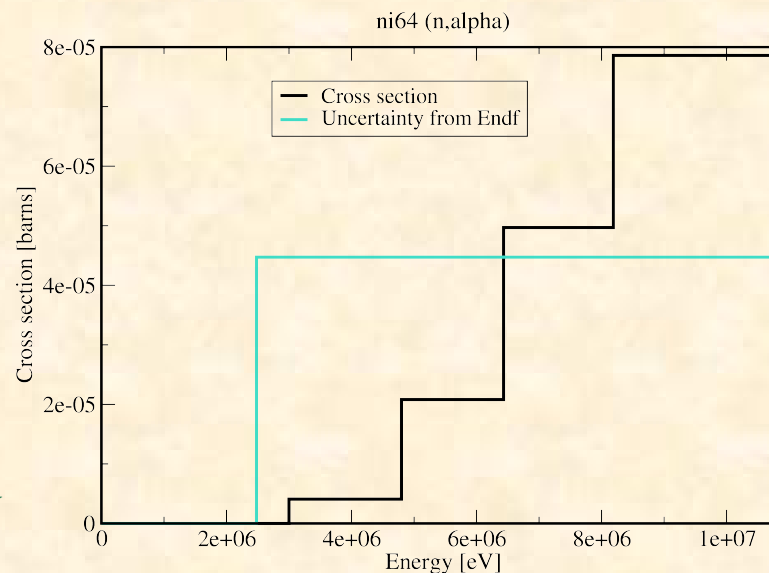 energy uncertainties are not available.

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

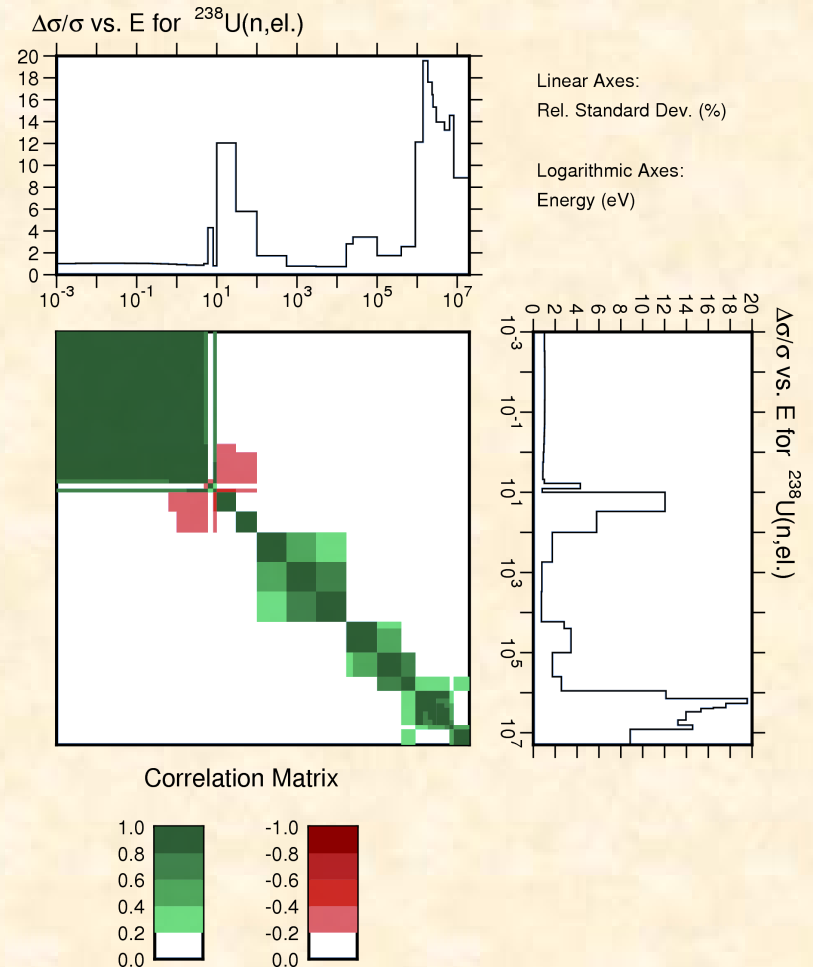Often for threshold reaction, for example Ni^{64} (n, alpha)
File 33 gives
- lb=0 or absolute covariance matrix
- additional section with relative covariance matrices

Uncertainty from lb=0
section only

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 lrf=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

$\Delta\sigma/\sigma$ vs. E for ^{238}U(n,el.)

Linear Axes:
Rel. Standard Dev. (%)

Logarithmic Axes:
Energy (eV)

$\Delta\sigma/\sigma$ vs. E for ^{238}U(n,el.)

Correlation Matrix

1.0	-1.0
0.8	-0.8
0.6	-0.6
0.4	-0.4
0.2	-0.2
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.

^{238}U
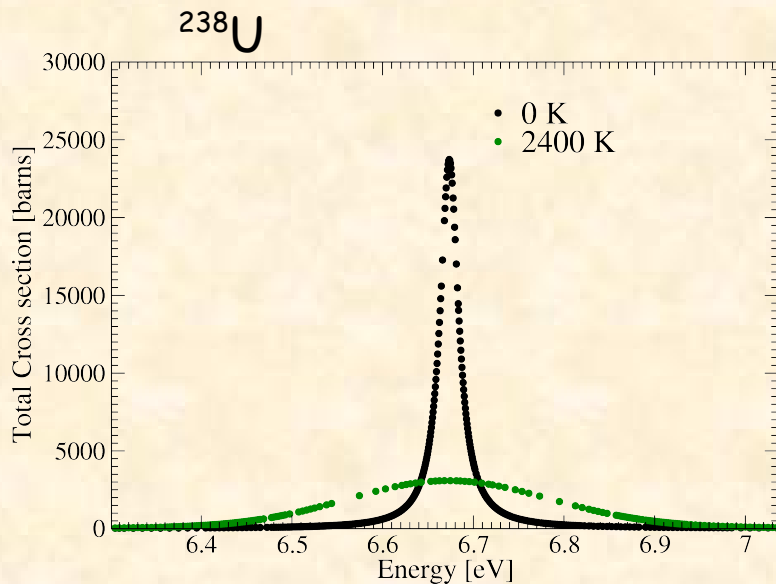
0 K: 1049356 points
2400 K: 42461 points

^{11}B
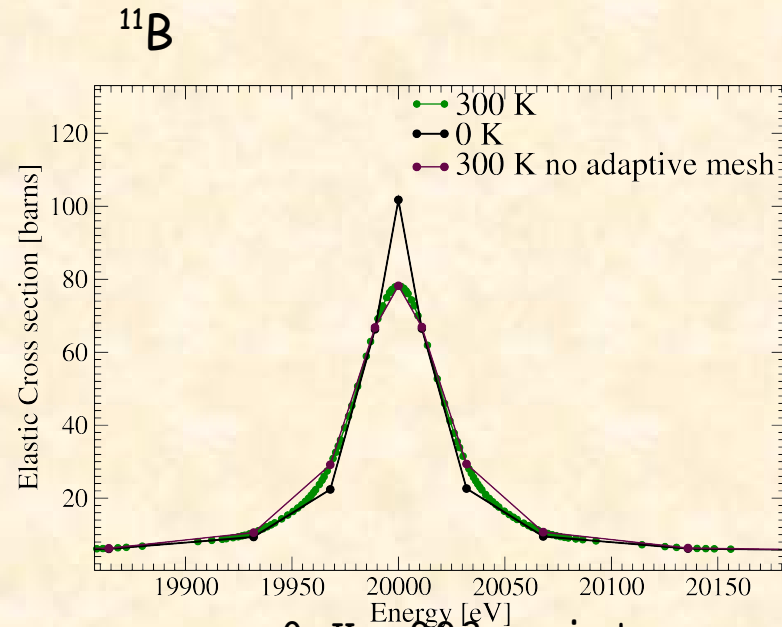
0 K: 993 points
300 K: 807 points

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.
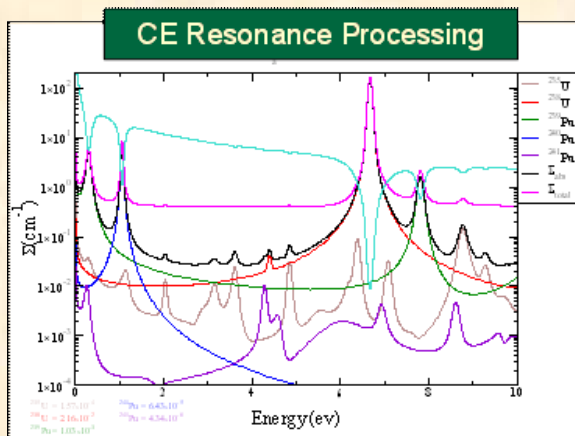
Most AMPX modules have automated test cases

```
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
```

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UT–BATTELLE

Exsite as future GUI for SCALE and AMPX

Allows to construct and run input files
Currently working only for selected SCALE programs
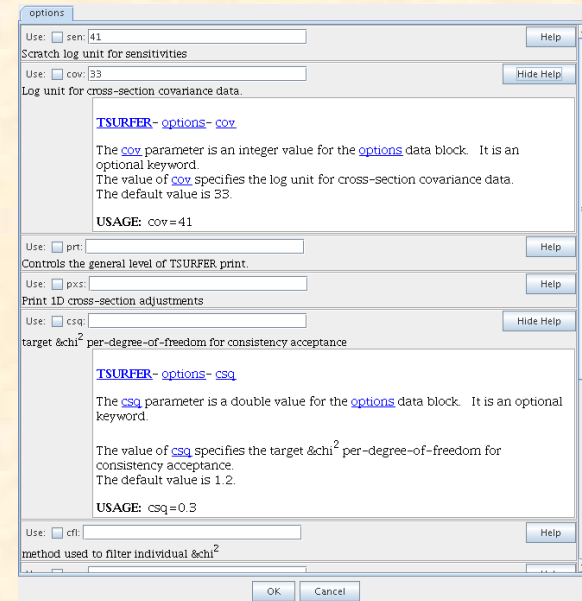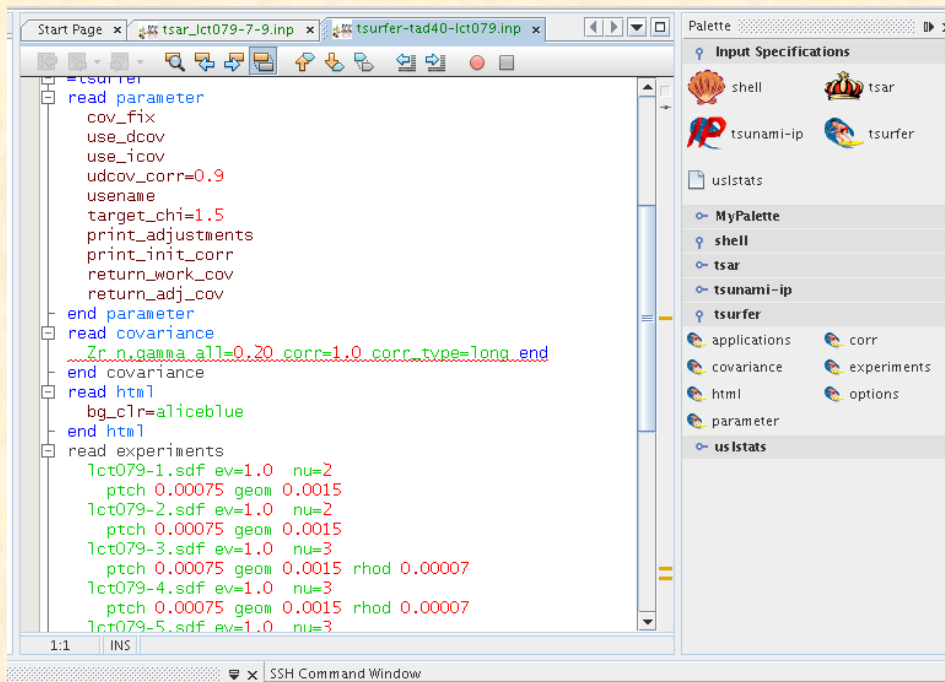
Exsite to run and compare benchmark results

can be used for MG and CE comparison

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Template engine to produce input files
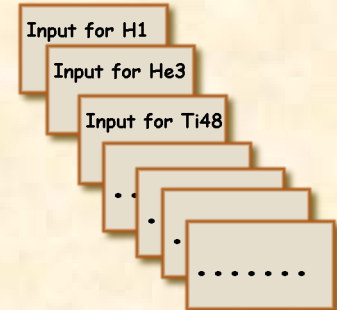
```
<Materials>
    <Material tag="h1"
            endf="125"
            za="1001"
            tape="n-001_H_001.endf"
            ...
        <Material tag="u238"
            endf="9237"
            za="92238"
            tape="n-092_U_238.endf"
    ...
</Material
```

+

```
<InputData>
    <openFile name="&batch;"/>
<loop restrict="+neutron(yes)">
    <openFile name="&case;"/>
        <writeFile name="&case;">

<text>=shell
ln -sf &broaden_file; ft34f001
end
=pickeze              <!-- pickeze -->
-1$$ 3000000
0$$ 34 35
```

Input for H1
Input for He3
Input for Ti48

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

Defines sequence
Uses a few user defined parameters

Plan to use in Exsite to support "SCALE-like" sequences

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)