AMPX Cross-Section Processing Status

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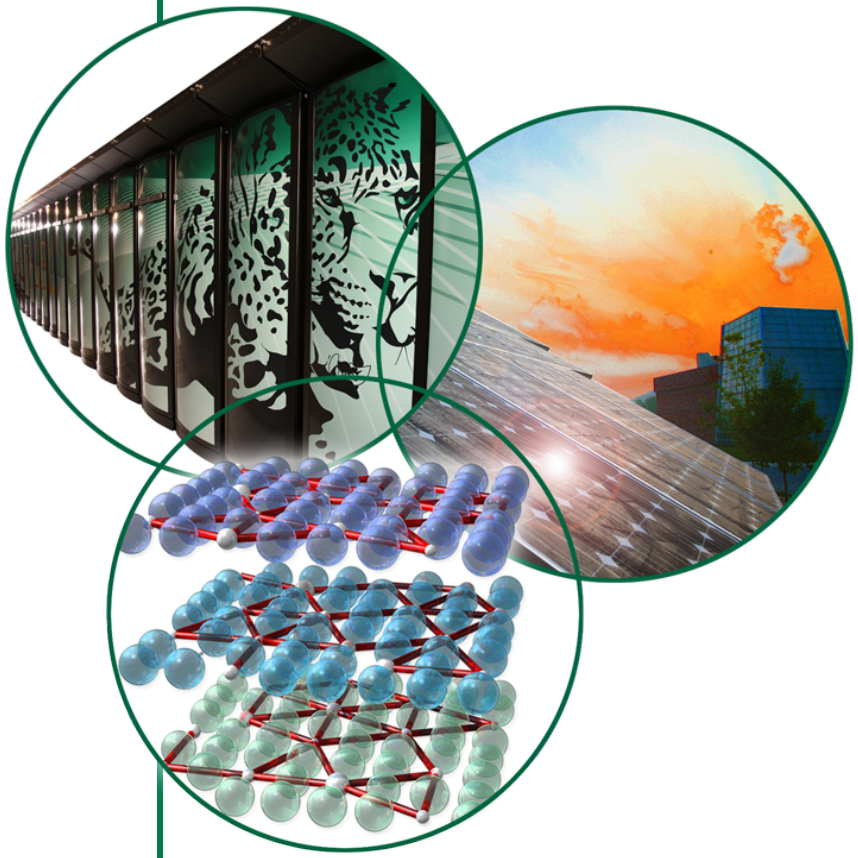
CSEWG MEETING



U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY

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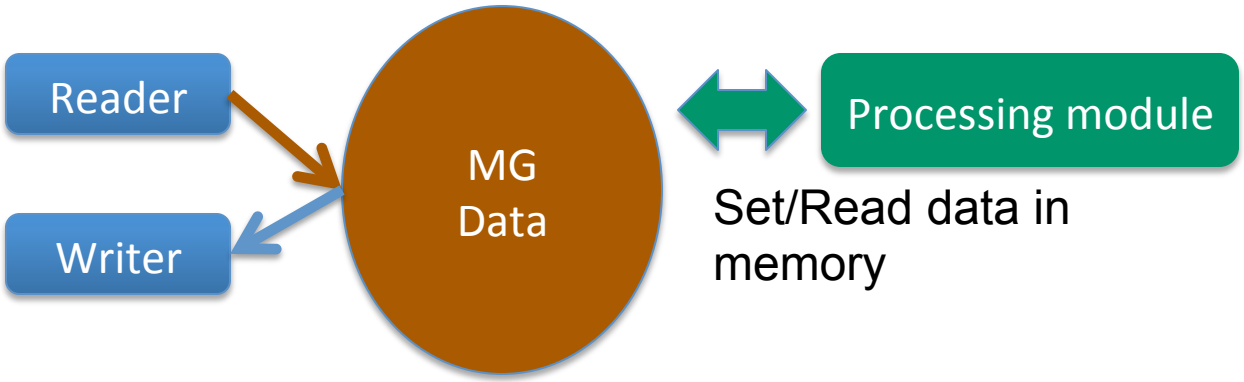
AMPX/SCALE repository merge

- Merge AMPX into the SCALE repository
- Convert to use the same build system.
  This allows developers to develop in the same frame work
- Easier to share components that are the same for AMPX and SCALE
- Can now use SCALE's test harness
- Will start to use the same QA procedure

Share MG Library Resource

SCALE developed a C++ in-memory resource to access MG library data.
Reader and Writer classes are provided.
Fortran bindings are provided.

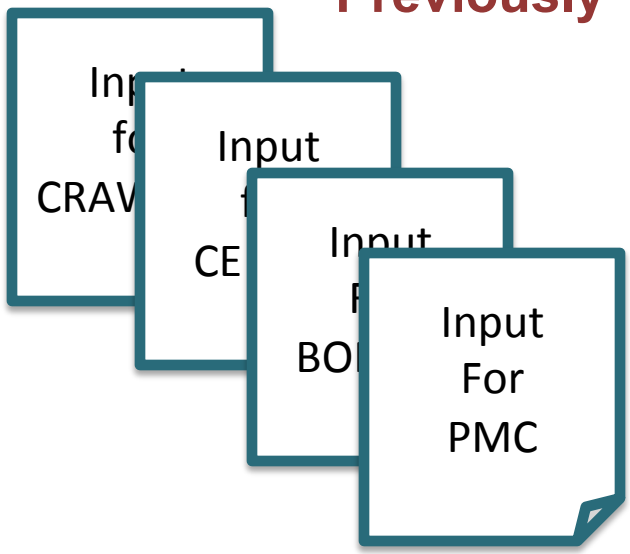


After the repository merge, AMPX can easily share the resource.
If file format changes, it “automatically” changes in SCALE and AMPX.
In-memory resource already allows for additional MG data (Subgroup data) and more than 999 groups.
Most of the AMPX modules have been changed to use the new resource (X10 is in the process of being changed).

In order to calculate LAMBDA factors and homogenous f-factors, we need to calculate shielded cross section using CRAWDAD, CENTRM, BONAMI, and PMC.

Previously

Generate Input



Run each module as separate program using system calls.

Updated version

Scale Shielding module

SCALE added new sequence concept where processing is done in memory.
AMPX now takes advantageous of the new shielding cross section module.
All data are passed in memory
Changes in module input will be propagated at compile time – no more writing input for each program

AMPX Modernization Efforts

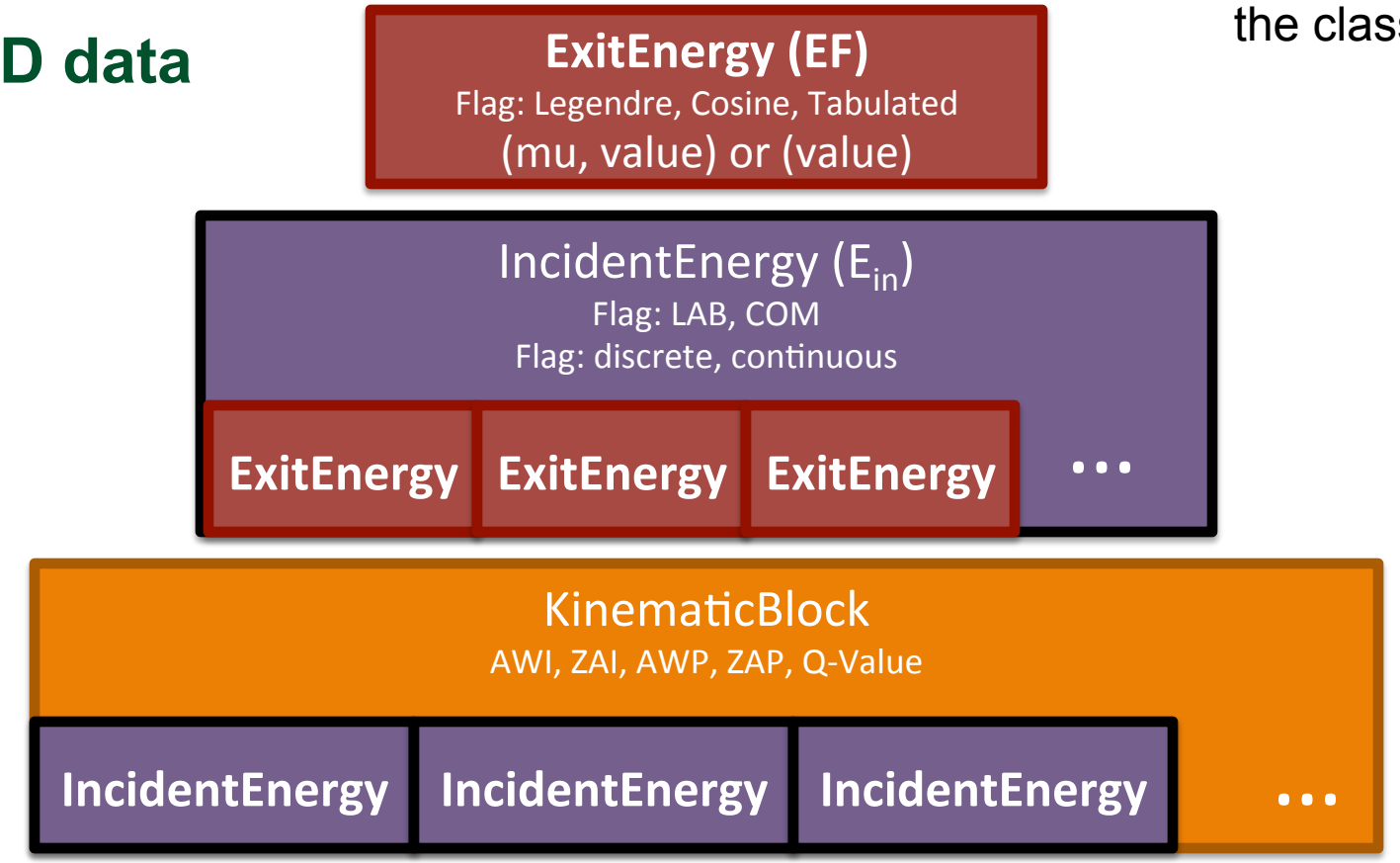
- ORNL received NCSP funding to modernize AMPX
- This allowed us to start major code updates
- New modules will use C++ to allow easy code reuse.
- We focused on Y12, our code to generate kinematic data since the current version cannot write out tabulated kinematic data. This is needed for thermal moderator data in CE libraries.
- Y12 needs many of the basic functionality given in the AMPX library functions, so many of the basic functionalities were rewritten in C++.

Basic Data Containers translated from Fortran to C++

1-D data

- Used in all new code
- Basic methods for integration and data access provided in the class

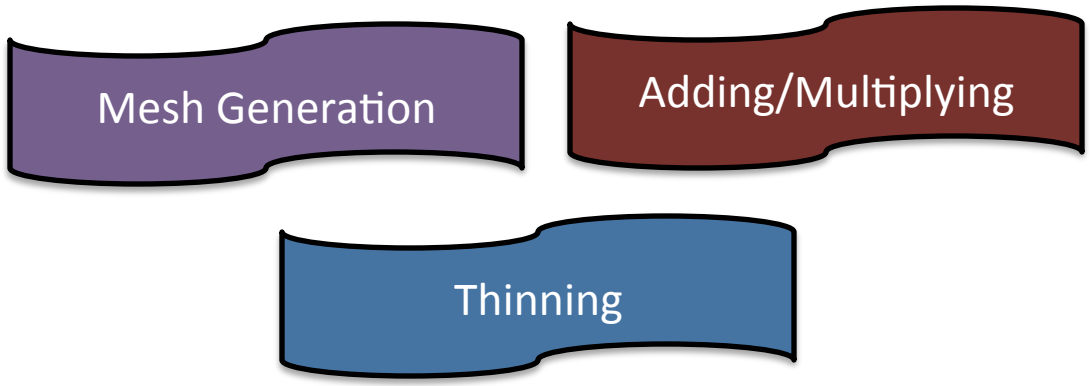
2-D data



C++ allows the use of templates and functions that operate on them
(we used templates instead of inheritance to ensure type safety)

Iterator
Remove
Insert
Interpolate
can interpolate ?

with this concept of an iterator we can define template functions to do the coding once.
Hard part is interpolation and equality check (see next slide)



- Provided an Iterator class for all data containers:
  - Tab1
  - ExitEnergy
  - IncidentEnergy
  - KinematicBlock
- Do most of the unit test on the template functions using 1-D data, as it is easy to test.

Interpolation and Equality test

On Energy in Tab1 or angular cosine in tabulated angular distributions:
just interpolate or compare on union grid – refine mesh as needed

On Exit energy:

- Only compare ExitEnergy objects given at the same exit energy.
  Now we only need to compare on angular cosine value or legendre order.
- Interpolate if needed before comparison.

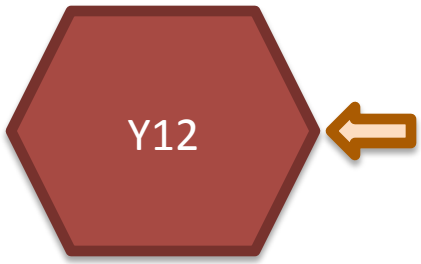
On Incident Energy:

- Interpolate using Unit-based interpolation.
  Corresponding point interpolation is supported, but internally AMPX uses Unit-based
- Only compare for the same incident energy.
  Interpolate before comparison if needed.

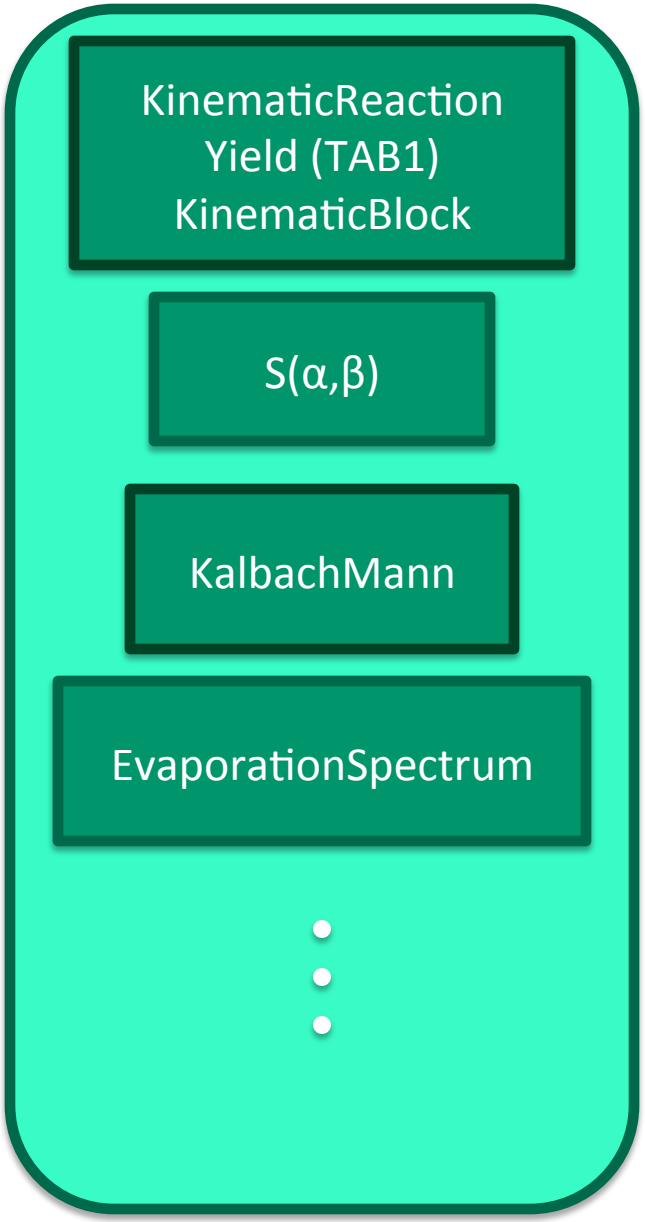
Note: Filling a mesh of incident energies based on a halving scheme can lead to an extremely dense mesh. Therefore we also allow a equality test based on exit energy range only.

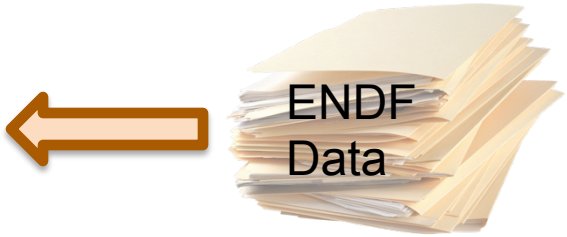
Processing code never reads ENDF formatted files directly

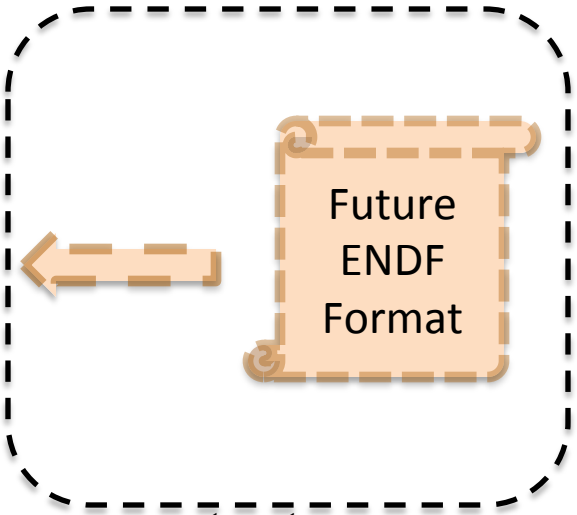
Y12 never reads ENDF data directly.



Produces:
Tab1
KinematicBlock







not yet implemented

Processing of Elastic and Discrete Inelastic 2D data

Given in ENDF as angular distribution for a given incident energy in COM.
Exit energy is given by kinematic formulas.
SCALE needs the data in LAB.
AMPX converts Legendre to tabulated if needed and then converts to LAB, finding a suitable exit energy mesh.
Additional incident energies are added for discrete inelastic reactions:

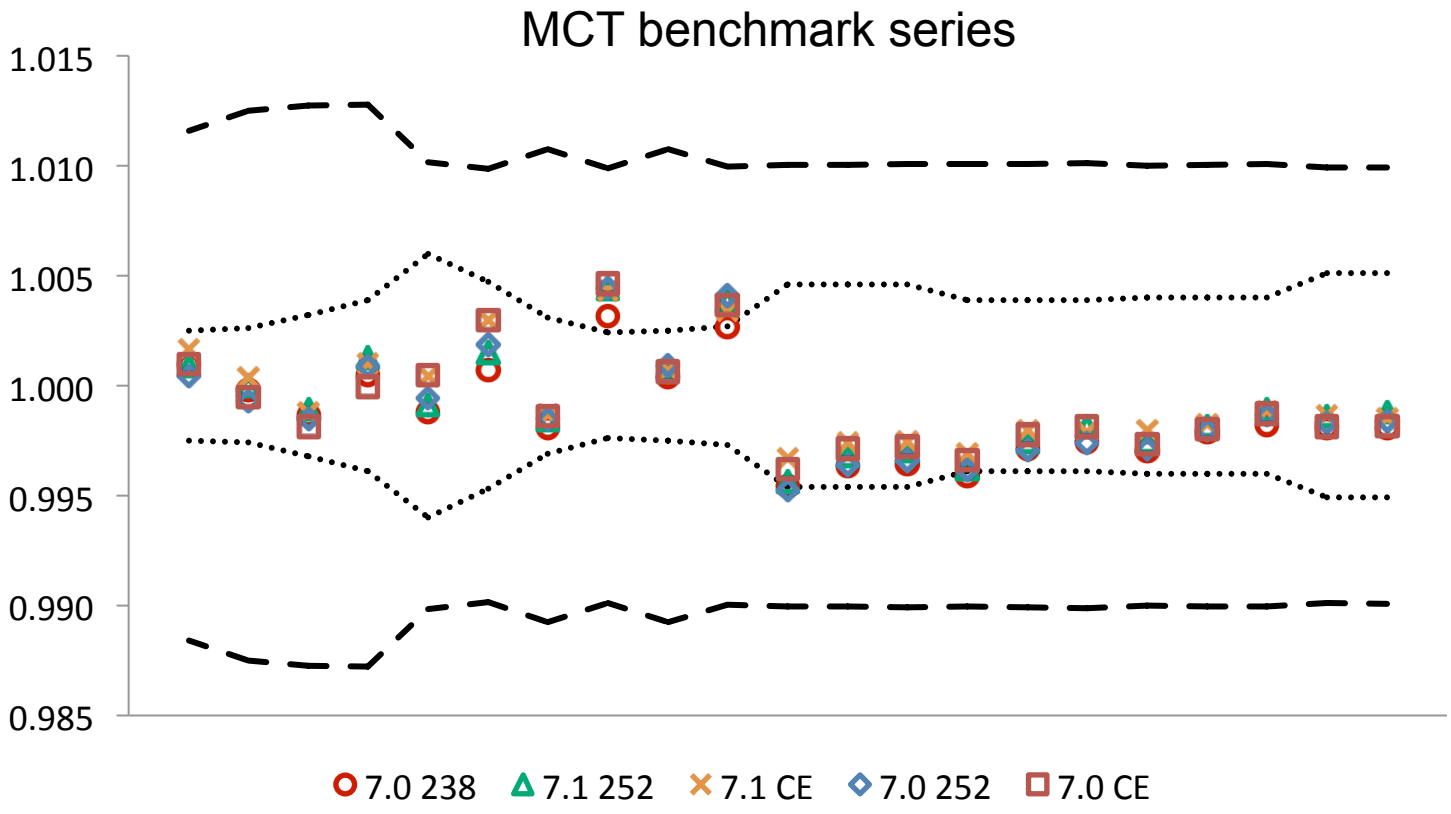
- Add 10 additional incident energy values between threshold and first incident energy given in ENDF (equal lethargy spacing).
- Refine the mesh (based on a halving scheme) over WHOLE incident energy range. HOWEVER, only ensure that the exit energy range can be interpolated in a unit-based interpolation.
- Thin the mesh, but compare for each incident energy, exit energy, and angle, i.e. the FULL distribution.

For AWR < 1, jacobian for angle has a discontinuity.
Add exit energies as close to discontinuity as numerical possible.

Since MG uses Legendre orders in LAB, discontinuity is not present, as angle jacobian is not needed, since we integrate over angle.

Generate ENDF/VII.1 library

Use the new Y12 to generate the kinematic data
Use the merged AMPX/SCALE repository version
Generate CE libraries, 252-neutron group and 200n/48g coupled library



Run extensive tests on the library (transmission and benchmark cases)

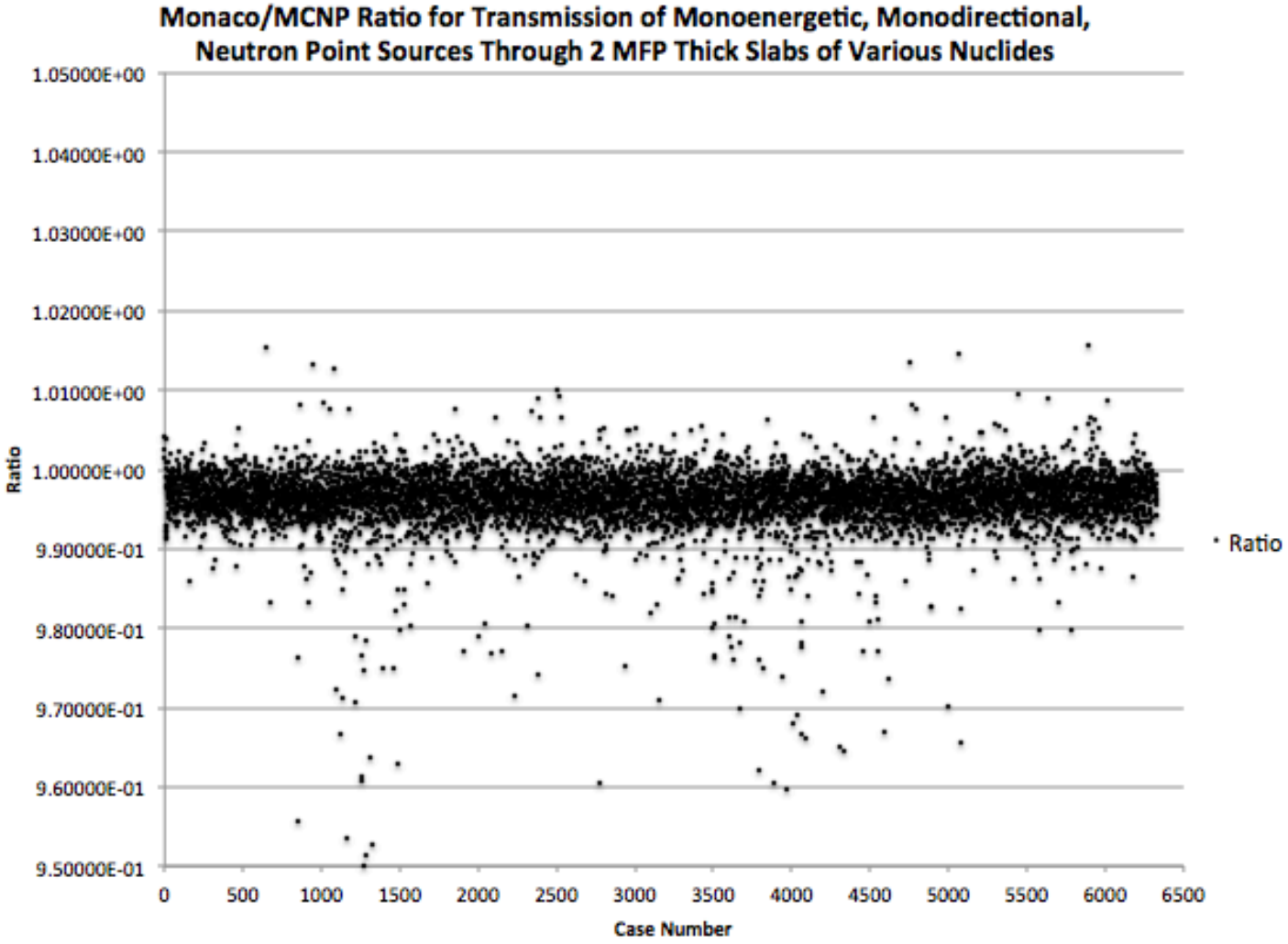
Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries

- Compared MONACO with AMPX-Generated CE Library to MCNP6 with NJOY-Generated ACE Library
  - Transmission Test Suite (7215 total cases)
    - Mono-energetic, Mono-directional, Point Source
    - 2 MFP slab of attenuating material
    - Compares total flux transmitted through slab to 2x2x2cm detector
    - Neutron-only (15 energies) and Gamma-only (9 energies) test suites
  - Leakage Test Suite (421 cases)
    - ^{252}Cf S.F. Neutron Spectrum, Point Source in center of 25cm sphere of attenuating material
    - Run in Coupled n-γ mode
    - Compares neutron and gamma leakage spectra at outer radius of sphere for all converged (R.E. < 5%) groups

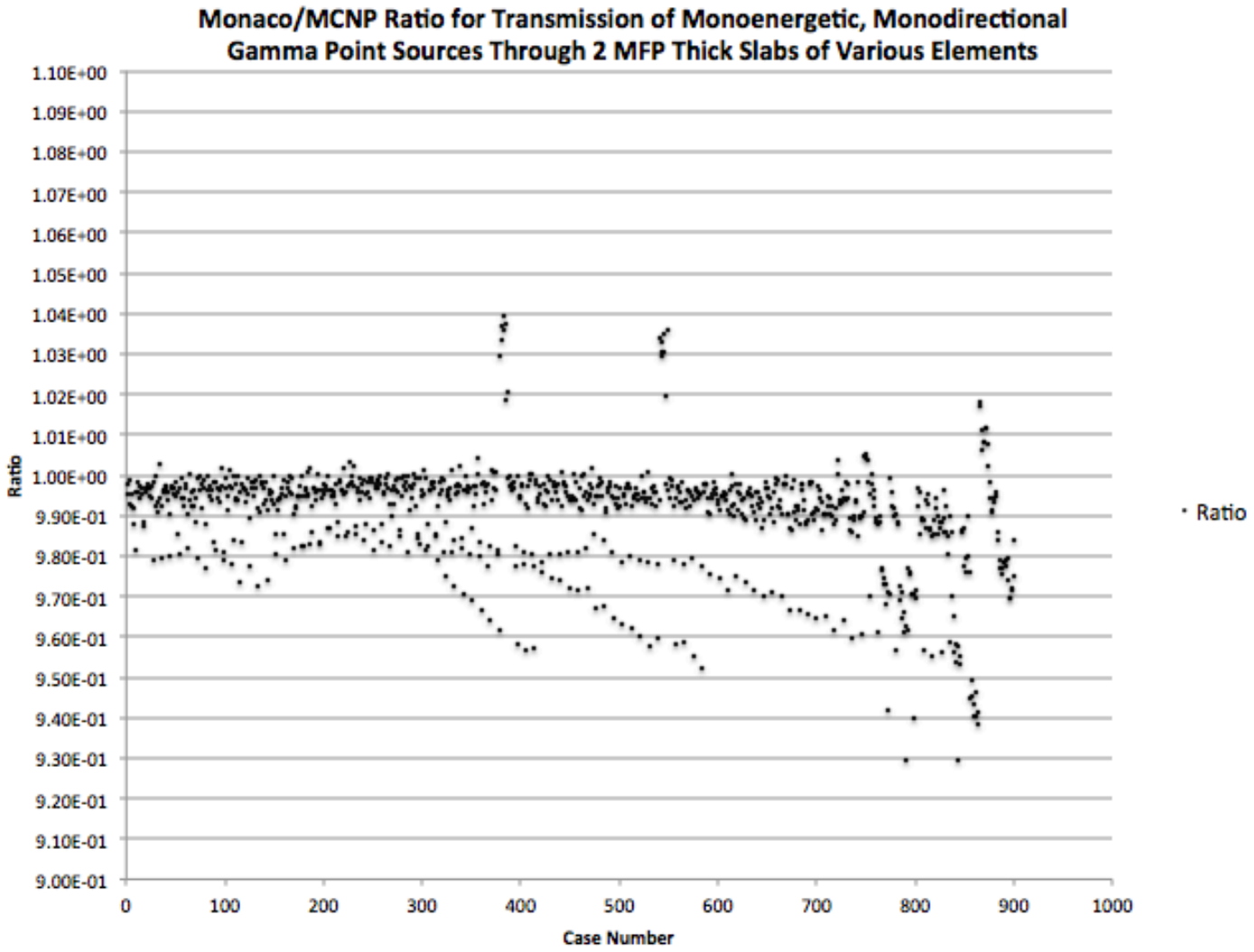
Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries

- 6315 Total Jobs in Neutron Transmission Test Suite
  - 421 Isotopes * 15 Source Energies
    - Does Not Include ^{22}Na or ^{7}Be
  - Source Energies at Mid-point of a Corresponding SCALE-200n47g Group
    - 14.0155, 10.2565, 5.0932, 3.87225, 2.9385, 1.96975 MeV
    - 982.12, 510.635, 104.56, 9.8569, 1.0976 KeV
    - 90.096, 9.4962, 1.02, 0.1125 eV
- 900 Jobs in Gamma Transmission Test Suite
  - 100 Elements * 9 Source Energies
  - Source Energies at Mid-point of a Corresponding SCALE-200n47g Group
    - 13.0, 9.0, 4.75, 1.1 MeV
    - 950.0, 511.0, 125.0, 52.5, 25.0 KeV
- 421 Jobs in Coupled Leakage Test Suite
  - 421 Isotopes * 1 Source Spectrum (^{252}Cf Spontaneous Fission)
    - Does Not Include ^{22}Na or ^{7}Be

Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries



Testing of ENDF/B-VII.1-Based Continuous Energy Cross Section Libraries



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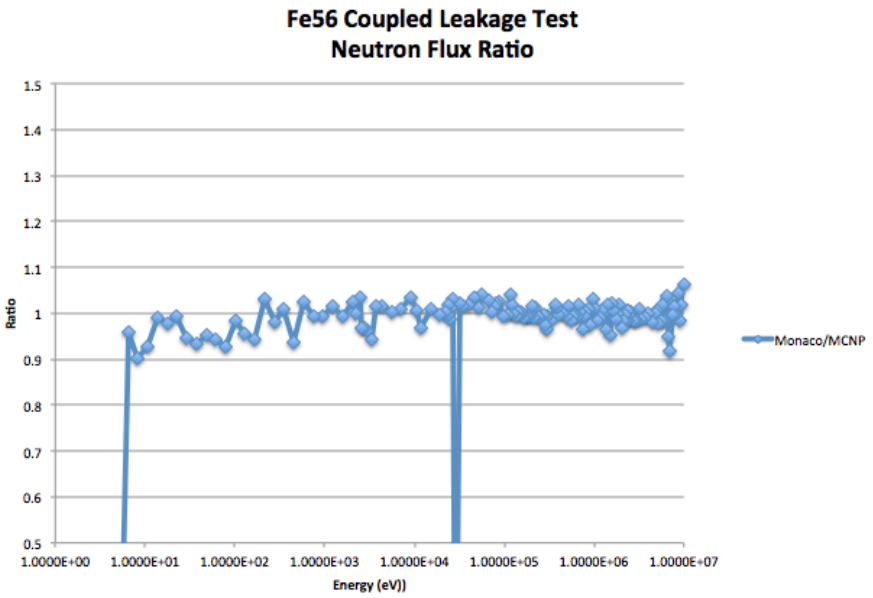

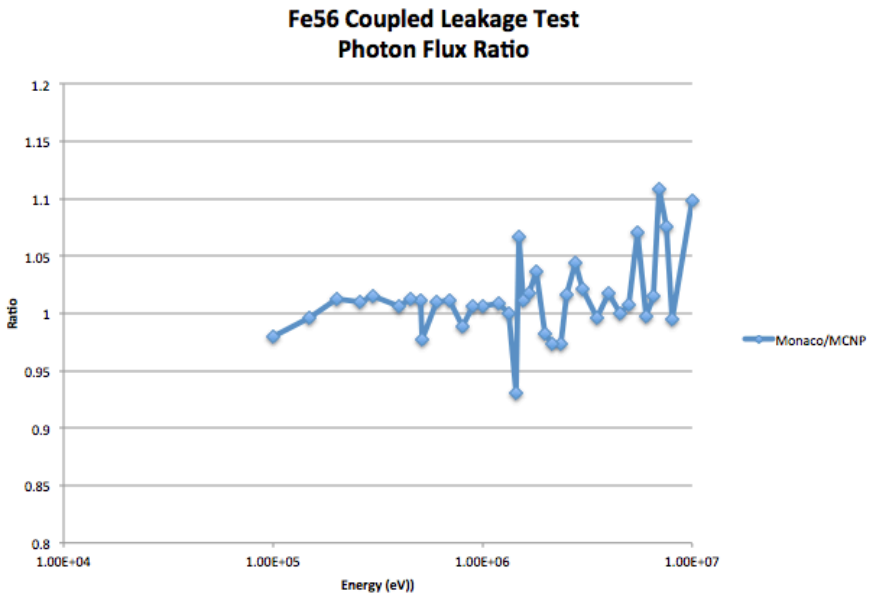

Summary

- Converted AMPX build system to SCALE build system
- Merged AMPX and SCALE repositories
- Started the AMPX modernization
  - Updated many of the foundation functionality to C++
  - Rewrote Y12 in C++ using the new foundation functionality
- Created CE and MG ENDF/VII.1 libraries using the modernized, merged AMPX code.
- The CE and MG ENDF/VII.1 are currently tested in SCALE for release with the SCALE 6.2 version.