

AMPX status report

D. Wiarda

A. M. Holcomb

S. W. Hart

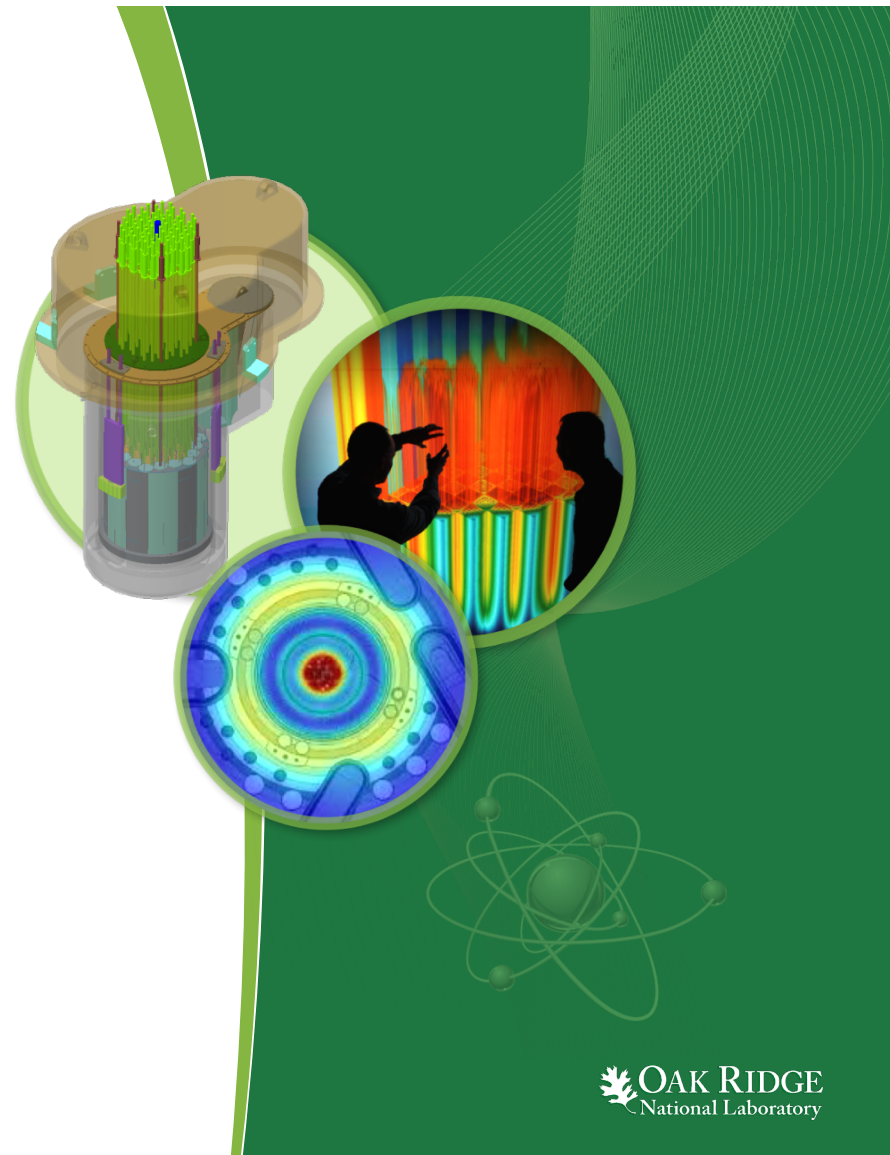
M. L. Williams

CSEWG

Brookhaven National Laboratory

Nov. 7, 2017

ORNL is managed by UT-Battelle
for the US Department of Energy



Introduction

- New continuous energy (CE) library format
- Modernization of Platinum
- Modernization of Jamaican
- Status of general nuclear database structure (GNDS) in AMPX
- Support for new evaluated nuclear data file (ENDF) formats

CE Resource

- SCALE is moving to a new binary on-disk format (HDF5 based) for the CE libraries.
- A new in-memory C++ resource for the library was developed (ROBUS), to be used throughout SCALE.
- The resource and the on-disk format is extendable to accommodate new types of data.
- Unfortunately, it cannot be used as-is in AMPX, as it does not allow changing of the data.
- Added an in-memory layer (CEResource) that transfers from and to ROBUS but allows updates
- Existing: Convert existing CE libraries to new format
- Planned: Convert new format libraries into current CE library format.

Iterator classes in AMPX

FillObject: basic class that must be implemented for all supported types. For example, 1-D adds a function returning the function value

FillObject

getE
setE
getInter
setInter

FillList: list of FillObject objects over which one can iterate. Supported types must implement the *interpolate* and *canInterpolate* functions

FillList

getNew(e)
getCurrent
Interpolate(e)
canInterpolate
start
advance
backspace
isEnd
insert
remove

FillAdvanceMultiple: a list of FillList objects over which one can iterate. Discontinuities are preserved and added at the beginning and end of the range of each FillList

FillAdvanceMultiple

start
advance
backspace
isEnd
getCurrentE

Union grid

- For the SCALE CE libraries:
 - Cross section data for all temperature independent reaction (51, 52, ..) are on the same energy grid. However, on-disk, a sub-set of that grid sufficient for the given reaction is stored
 - Cross section data for all reactions for a given temperature are on the same grid. This grid must include all energy points from the union grid of the temperature-independent cross section data
 - In the CEResource, all reaction data are given for each temperature. If data are the same across temperatures or reactions, C++ smart pointers are used
- For the 1-D data in the CEResource, an implementation of the iterator classes was provided
- This makes it easy to generate the union grids. Additional functionality was added to allow data thinning on the union grid and to require certain points on the union grid

Calculation of redundant cross section data

ReactionResource



- SCALE and AMPX share a ReactionResource class
 - contains an mt value for each reaction
 - Includes multiplicity if applicable
 - if redundant, reactions to be added to calculate the redundant cross section
- A template class allows for calculating the redundant cross section. Implementing classes need to provide:
 - exist(mt): check whether the reaction exists
 - getCross(mt): obtain the data for the desired reaction
 - addCross(mt): add the new reaction data
 - remove(mt): remove the reaction data

A class was added to recalculate the redundant cross section data in the CEResource. This assumes that the cross section data are on the correct union grid.

Platinum

- An AMPX module was developed to bind the final CE library from:
 - Cross section data
 - Kinematic data
 - Probability tables
- The modernized version is entirely written in C++ and uses CEResource to:
 - Store the data on-disk
 - Create the necessary union grids
 - Resume redundant cross section data
 - Ensure that 1-D and 2-D end at the same energy points
 - Updated user input is included

Jamaican

- Jamaican is an AMPX module to convert double-differential kinematic data into cumulative probability distributions for use in CE calculations
- All distributions are in laboratory system and tabulated form; if not, then Jamaican uses existing AMPX routines to convert
- Y12 sorts double-differential data first by incident energy, then by exit energy, and finally by angle; CE libraries need a marginal probability distribution in angle and a conditional probability distribution in exit energy for each incident energy
- AMPX iterator classes are used to generate and thin the union grid of angles for each incident energy

Jamaican architecture

Bragg-Edge
Distributions

Bragg-Edge

Base class

Reaction info

Calculate equiprobable
angles

Obtain the distribution in
Jamaican format

Elastic

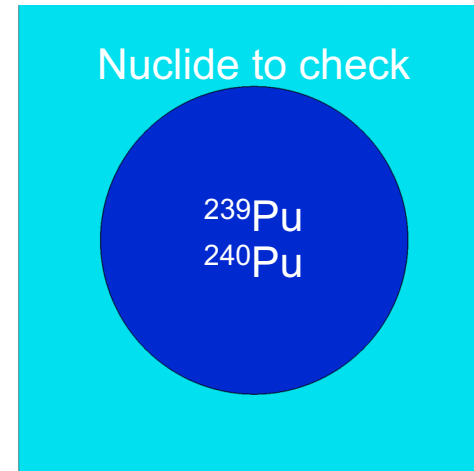
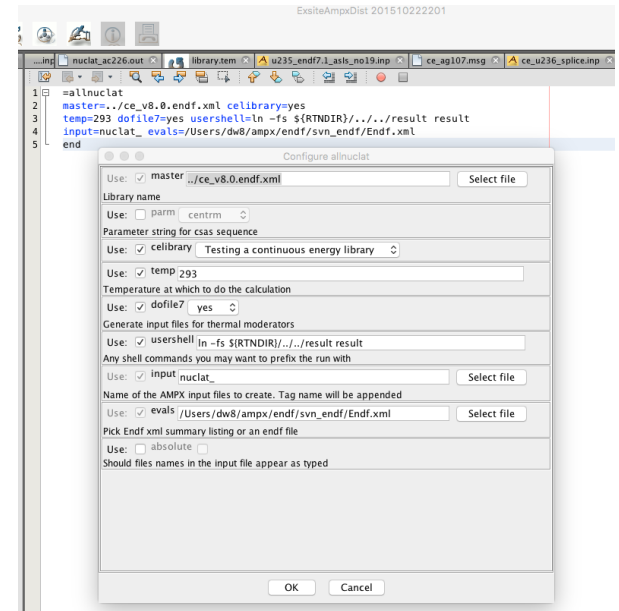
Continuous in
angle and energy

Discrete exit
energies
(Gammas)

- Implementation in C++ allows a more modular design
- Division into base class and child classes for different types of distributions allows code to be shared

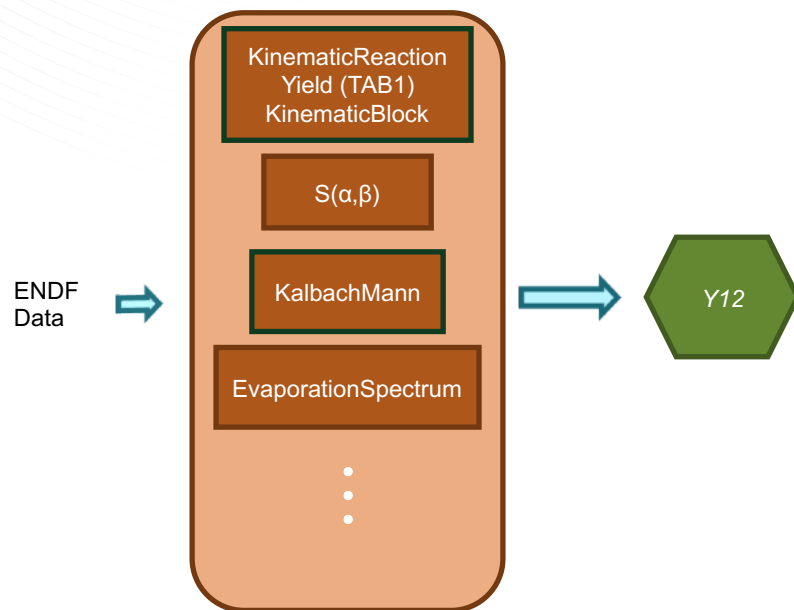
Testing of Platinum and Jamaican

- Generate ENDF/B-VIII.0 library with current version and modernized version of Jamaican and Platinum
- Run KENO for a pin-cell with a moderator substituted by each nuclide in the library (ExSite can generate the input files)
- Compare between current and modernized version
- Note that the hard spectrum for most nuclides allows testing for anomalies for the threshold reactions
- Run the VALID suite



GNDS

- AMPX has code for low-level containers
- Work continues to add the GNDS on top of that



- GNDS data will be read into existing in-memory AMPX structures for further processing
- Most AMPX codes that read ENDF data already use those in-memory structures instead of reading ENDF directly

AMPX modernization

Module	Functional Capability	Estimated Completion Data
PUFF	Generate covariance data from ENDF/B evaluations	Finished
POLIDENT	Generate 1D CE data from ENDF/B evaluations	Finished
JAMAICAN	Produce CE collision kinematics PDFs and CDFs for Monte Carlo libraries	Finished
PLATINUM	Assemble CE library for Monte Carlo calculations	Finished
BROADEN	Doppler broaden 1D CE data	12 month

Probability tables

- MET-1000
 - single cube, homogenized assembly with reflected BCs
 - room temperature
 - fast spectrum
- Codes
 - MCNP v6.0
 - KENO v6.2

ENDF	Model	MCNP	KENO-STD	Δ KENO-STD (pcm)
VII.1	MET1000 – Add. – C1	2.11970	2.12569	-599
	MET1000 – Add. – C3	1.00518	1.00580	-62
	MET1000 – Hom.	1.29718	1.30185	-467
	MET1000 – Het.	1.29523	1.29941	-418
	MOX3600 – Hom.	1.15822	1.16436	-614
	MOX3600 – Het.	1.14381	1.14964	-583

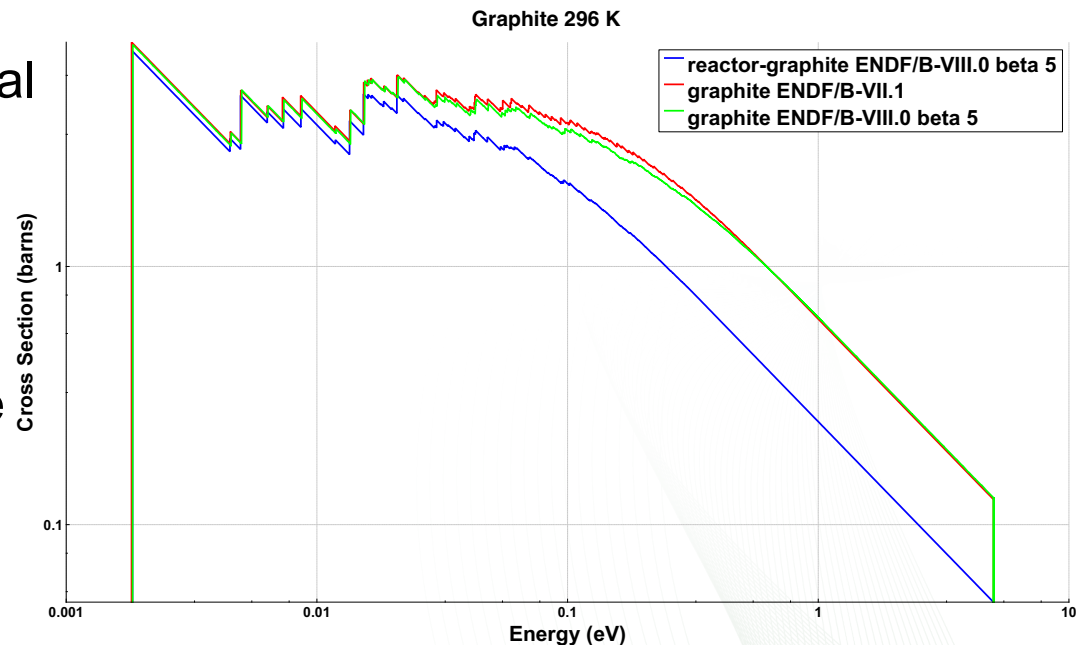
Probability tables (continued)

- The ENDF prescription for URR reconstruction:
 - Multiplicative: results from probability table construction are meant to give cumulative distribution function (CDF) shapes only, and so they are to be normalized and then scaled by a smooth cross section (given in File 3)
 - Additive: a background cross section (from File 3) is to be added to probability table values
- NJOY renormalizes **additive** tables to values calculated with J-functions
- Add an option to Purm to renormalize.

ENDF	Model	MCNP	KENO-STD	KENO-NEW	Δ KENO-STD (pcm)	Δ KENO-NEW (pcm)
VII.1	MET1000 – Add. – C1	2.11970	2.12569	2.11905	-599	65
	MET1000 – Add. – C3	1.00518	1.00580	1.00467	-62	51
	MET1000 – Hom.	1.29718	1.30185	1.29706	-467	12
	MET1000 – Het.	1.29523	1.29941	1.29473	-418	50
	MOX3600 – Hom.	1.15822	1.16436	1.15793	-614	29
	MOX3600 – Het.	1.14381	1.14964	1.14346	-583	35

Graphite

- SCALE CE library distributions:
 - are in the lab system
 - are marginal in angle and conditional in exit energy
 - no discrete angles
- For coherent elastic scattering, this means there are two angles for each angle given in ENDF for at least all the incident energies given
 - ENDF/B-VII.1
 - graphite: 248 incident energies
 - ENDF/B-VIII.0 beta 5
 - graphite: 2,379 incident energies
 - reactor-graphite: 530 incident energies



Fission Energy Release

- AMPX does not yet store the Fission Energy Release in any library
- However, code need to be changed to jump over the TAB1 record if present.
- AMPX reads the entire File 1 information into memory and therefore even codes that do not use the energy release section in File 1 may fail.

New P(nu) format

- No space is available for the data on any SCALE library
- ENDF reading routines have been changed to add a distribution with -1800n (n= 0,1,..) for neutron and gamma containing:
 - Yield data
 - Double differential data either copied from File 5, File 15, or as given in File 6 if LAW is not equal to -5 or -15
- All processing codes ignore kinematic data if corresponding 1-D are not present (current version of Platinum had to be changed to not write it to the library)
- Added routines that check yields of all -1800n reactions sum up to 1. If exit particle is a neutron, total nubar must be checked to ensure that it is consistent with the yields
- If distributions for the total are not given in the ENDF file, the total must be recalculated
- ToDo: test the new ENDF routines and add unit tests

Summary

- The AMPX modules Platinum and Jamaican were modernized
- Support for the new P(nu) format has been added, but data are not yet used in SCALE
- Initial support for the new fission release format has been added, but data are not yet used in any SCALE library
- The new features are expected to be available in SCALE 6.3
- A SCALE 6.3 beta is expected in March 2018