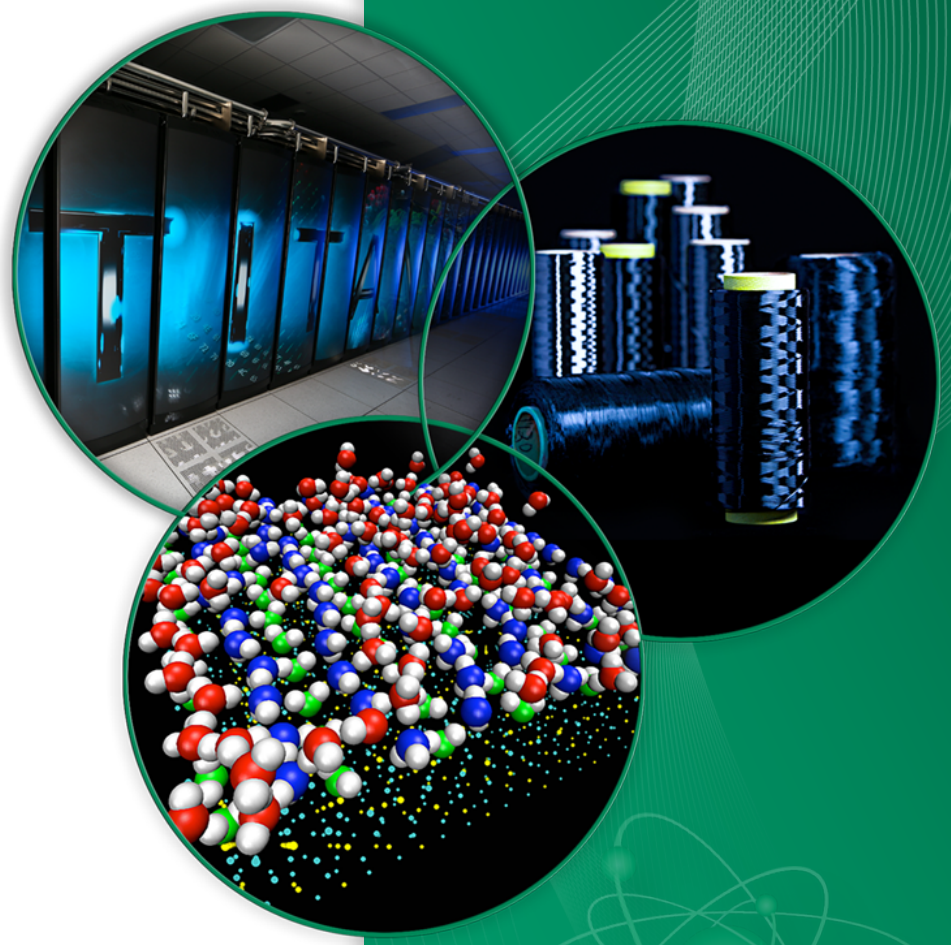
QA Discussion



Michael Dunn

WPEC Subgroup 38 Meeting

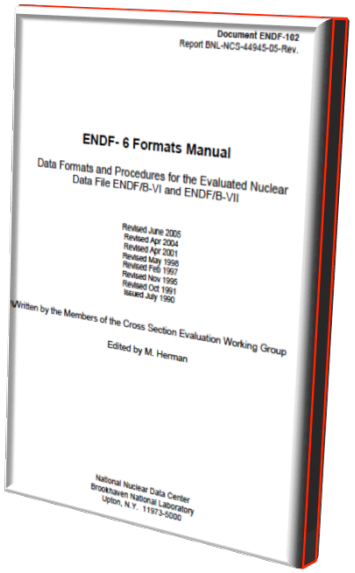
December 9-11, 2013

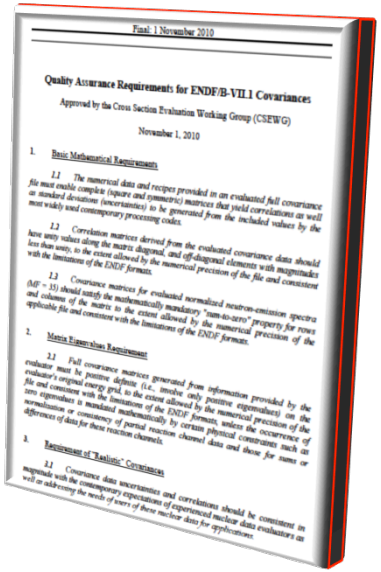
Quality Assurance Plan and Procedures

- Mission
  - Develop and implement the quality assurance (QA) infrastructure, which ensures QA requirements are verifiably met and is as low-impact as possible, to support the development, deployment and maintenance of a new, modern international database format/ structure.
- Goals (Tasks):
  - Determine the QA requirements
  - Develop the QA plan (QAP) with implementing procedures
  - Determine and implement the testing requirements to support the QAP implementation and ensure QA
  - Develop and deploy the infrastructure needed to provide QA to the nuclear database—continuous integration model

Needs and Wants

- Sponsor and/or end-user requirements
- Annual assessment is required
- Graded / scalable
- Low-impact / integrated
- Modern / best industry practices
  - NQA-1 Part IV Subpart 4.2 “Guidance on Graded Application of Quality Assurance (QA) for Nuclear-Related Research and Development”
  - ISO-9001
- Take credit for what we are already doing
  - ENDF-102 manual and procedures developed over the past 50+ years —a lot of lessons learned and do not want to repeat past mistakes
  - Established checking and processing codes
  - Validation Committee testing
  - ADVANCE – in development at NNDC
- Note: The QA plan is not the end result

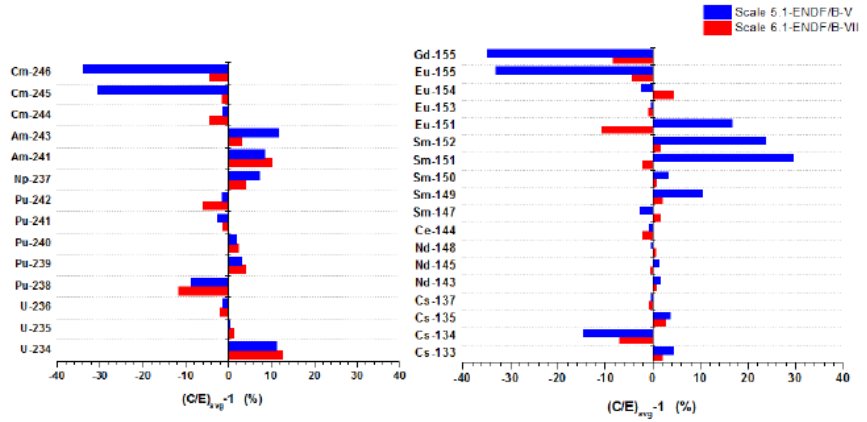




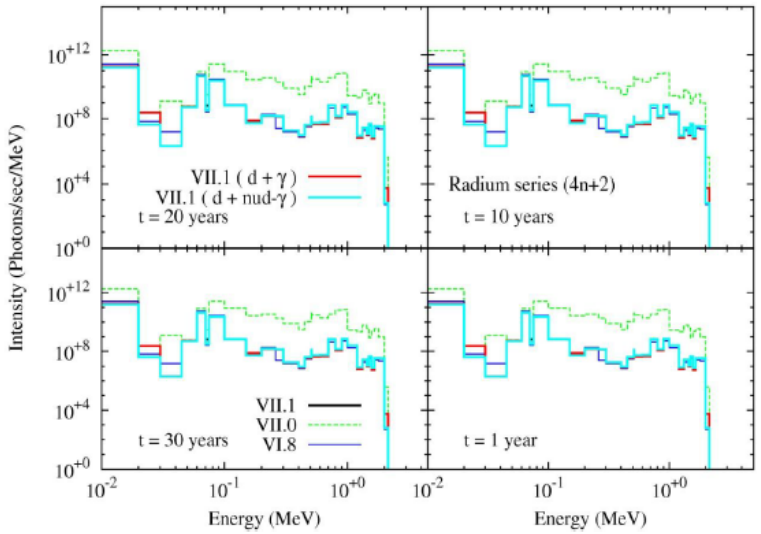
Build and Test Infrastructure

- Three types of testing – need comprehensive coverage
  - Unit Testing – low-level containers and API level
  - Regression – Verification tests performed on database to ensure integrity of database as commits come in (e.g., matrix summations, mass/energy balances, ADVANCE at NNDC, etc.)
  - Validation and Verification – For ENDF happens now at the Validation Committee (also could include ADVANCE here as well)
- Team tasks:
  - Identify and determine the tests needed
  - formalize and document each phase of testing (e.g., through project dashboard reporting—implement on GForge)

Isotopic validation – ENDF/B-V and -VII



Radium decay series (4n+2)



SCALE Example for Test Harness and Dashboard

- After every update, SCALE is automatically built and tested to ensure functionality of all tested features
  - ~500 test cases (still need more)
  - Linux, Mac, Windows
  - Intel and GNU compilers
  - Release and Debug mode

Linux Regression

Site	Build Name	Update		Configure			Build			Test				Build Time	Labels
		Files	Min	Error	Warn	Min	Error	Warn	Min	NotRun	Fail	Pass	Min		
node16.ornl.gov	LEGACY-RELEASE-Intel-12.0.3.174	13	0.2	0	0	1.3	0	0 -16	5.6	0	4	477	221.6	2012-03-07T11:50:42 EST	(none)
node16.ornl.gov	LEGACY-RELEASE-Intel-12.0.3.174	11	0.4	0	0	3.4	0	16 +16 -30	14.1	0	4	477	223.8	2012-03-07T07:48:54 EST	(none)

Quality Assurance Tasks

- Tasks defined at May 2013 WPEC SG38 Meeting:
  - Determine the QA requirements
  - Develop the QA plan (QAP) with implementing procedures
  - Determine and implement the testing requirements to support the QAP implementation and ensure QA
  - Develop and deploy the infrastructure needed to provide QA to the nuclear database—continuous integration model
- Goal for this meeting: determine the tests that need to be implemented
- Tests
  - Low-level containers – define unit tests
  - Physics tests: define regression tests
  - Library as whole: validation tests

Quality Assurance Tests

- Unit tests - low-level containers and API
  - Low-level containers and use cases still being discussed
  - Need to finalize low-level containers and APIs then work on unit tests—once in place
    - Can define “common” unit tests based on structure (e.g., container contents with numeric data conform to IEEE754 requirements)
    - Once use case is defined, can define unit tests that are geared toward intended use – if it is supposed to be a duck, test that it’s a duck
- Regression tests – physics tests (focus of next slides)
  - At this stage, we know many of the capabilities we want in the database (e.g., maintaining the existing ENDF functionality)
  - Should be able to compile list of tests that need to be implemented
- Validation tests – benchmarking and integral testing
  - Need to engage Validation Committees from different data projects to define more comprehensive unit tests (e.g., In US need to expand beyond criticality testing)
  - Efforts in progress now outside of SG38 effort, but could be a discussion for a later SG38 meeting

LLNL Physics Tests Implemented in Fudge

Partial list of tests from C. M Mattoon et. al. Nuclear Data Sheets:

Test	GND element
Are any errors encountered during resonance reconstruction?	reactionSuite
For each complete reaction (see Sec. V E), do Z and A balance?	reaction
Does the Q-value agree with value computed from particle masses?	reaction
Do errors appear when computing average energy/momentum for products?	reaction
Does energy balance (sum of energy deposited to products equal to incident energy plus Q)?	reaction
Is the cross section threshold consistent with the Q-value?	crossSection
Does the cross section span the interval from threshold up to the maximum (default maximum=20 MeV)?	crossSection
Can the cross section nativeData form be converted to pointwise, linearly interpolable form?	crossSection
Does the cross section contain any negative values?	crossSection
Do all 'transportable' particles have distribution information?	product
Are any product multiplicities negative?	multiplicity
Does multiplicity domain agree with cross section domain?	multiplicity
Does distribution domain agree with cross section domain?	distribution
Do distribution frames make sense (lab vs. center of mass)?	distribution
Are distributions normalized?	distribution
Are any probabilities less than 0?	distribution
Does the matrix have any negative eigenvalues? Is the variance positive?	covarianceMatrix
Does the matrix have very small eigenvalues?	covarianceMatrix
Are variances (diagonal of the matrix) unreasonably large or small?	covarianceMatrix

LLNL Tests Implemented in Fudge (continued)

- Since multiple resolved resonance regions are deprecated, warn if more than one is encountered. Now that Pu239 resonances have been updated, this one doesn't show up in ENDF-VII.1 anymore
- In URR, warn if the energy grid isn't dense enough (I think it warns if fewer than 10 points / decade are found in the file)
- Check Wick's limit (relating the size of elastic and total cross sections)
- For a threshold reaction, check that the cross section at (and below) threshold == 0.
- Check that 'summed' cross sections like MT1, MT4, etc. agree with the sum of their parts

LLNL Tests Implemented in Fudge (continued)

- Check that fission energy release is 'reasonable'—implemented because the polynomial expansions used to store fission energy release for many actinides were calculated in MeV, and only the 0th-order coefficient was converted to eV when storing in ENDF.
- For fission we don't have enough information to do a complete energy balance check, but we do now check that the energy deposited to neutrons + gammas is 'reasonable': no more than 20% of total energy available since the fission products must take some.
- If an Exception is raised at any point during the physics testing, we convert that into a warning rather than crashing.

ORNL Tests Implemented in AMPX
Input from Doro Wiarda

- Philosophy: AMPX is not a checking code; however, tests have been out of experience and necessity to catch "common" problems during library generation
  - Side comment: processing codes should not become checking codes; rather need checking codes/tools at the datacenters
- Kinematics distributions
  - Checks for inconsistency between 1D data and 2D data: threshold values for 1D and 2D are made to agree by assuming the 2D data are correct
  - Q-values are assumed to be correct and cross sections below the threshold are assumed to be zero
  - However, if the kinematics data for a threshold reaction are given in the COM, we ignore the distributions calculated below the threshold (calculated from the Q value)
  - 1D and 2D data are processed in the range given in the ENDF file and cut at the desired upper limit of the library (i.e., 20 MeV for reactor physics, shielding and criticality safety libraries)
    - Do not flag evaluations like ENDF/B-VII.1 Be7 that do not extend to 20 MeV; rather, AMPX fills the upper energy range for Be7 with zeros

ORNL Tests Implemented in AMPX

- Negative cross sections and kinematics data
  - Provide warning for negative 1D cross-section data but not negative kinematics distributions
  - Negative cross sections are set to zero
  - For CE libraries, negative 2D distributions are set to zero and 2D data are normalized after processing
  - For MG libraries, only set negative 2D distributions to zero if converting to tabulated format; otherwise, pass through as is (again emphasis is to be as faithful as possible to the original evaluation)
- Covariance matrices
  - Check for negative matrix eigenvalues and provides warning if negative
  - If diagonal elements are negative, we set to zero and provide warning
  - If File 2 and File 32 are out of sync, the PUFF module prints an error message but tries to continue processing and rescue what it can
  - Additional inconsistency checks are performed and alerrts the user if processing is not possible (e.g., cross material covariance matrices but no covariance provided for reference material)

ORNL Tests Implemented in AMPX

- AMPX has MG checking module (neutron and coupled neutron-gamma): RADE
- RADE performs verification tests at each step of the MG library generation effort – consistency checks for processed library but also provides check of underlying evaluated data
  - Checks for cross-section positivity
  - Verify the sum of the partials equals the total
  - Verify the sum of the elements in the MG transfer matrix (2D data) equals the corresponding 1D values
  - Performs many more consistency checks on MG data

ORNL Suggested Tests for Depletion & Decay Data
Input from Ian Gauld

- Ensure sum of decay branches is unity
- Verification against previous baseline would be a good idea (both at regression level and benchmark validation level)
  - Such testing would likely have caught the errors in ENDF/B-VII.0 decay library because there were so many huge changes that didn't make sense.
  - Challenge is that changes would then have to be confirmed against baseline—perhaps there could be some threshold to verify only large and unexpected changes.

ORNL Suggested Tests for Depletion & Decay Data

- Consistency check of delayed energy release per fission (included in main ENDF/B evaluations – File 3/8?) against decay energy using fission yields and decay energy for each nuclide.
  - This can be done using cumulative yields and decay energy Q easily without an ORIGEN-type calculation.
  - The problem here is that ENDF/B has not required consistency here, whereas JEFF has done more in this area to ensure consistency.
  - Another problem is that cumulative yields depend directly on the decay data. However, while decay data have been updated several times, there has been no parallel effort to revise the cumulative yields.
  - This is a big weakness is current ENDF/B data – our inability to regenerate new fission yield data as new decay data are developed.

ORNL Suggested Tests for Depletion & Decay Data

- Consistency check between energy in gamma line evaluations and energy from Q value. Again, these are currently known to be inconsistent for many nuclides, but this check could still be useful to see if situation is improving.
- Other code-based checks could be implemented, such as setting up simple decay chains. We did this for actinide chains after the last round of problems with the ENDF/B-VII.0 decay library
- Comment on depletion & decay validation benchmark testing
  - In recent years, ENDF has not performed a lot depletion and decay testing relative to criticality safety benchmarks
  - Validation Committees should use the fission pulse decay heat benchmarks that are some of the best (test decay and yield data)

Next Steps

- Collect additional checks/tests from NJOY, NNDC checking codes, etc.
- Develop list of additional regression tests by SG38 WG….