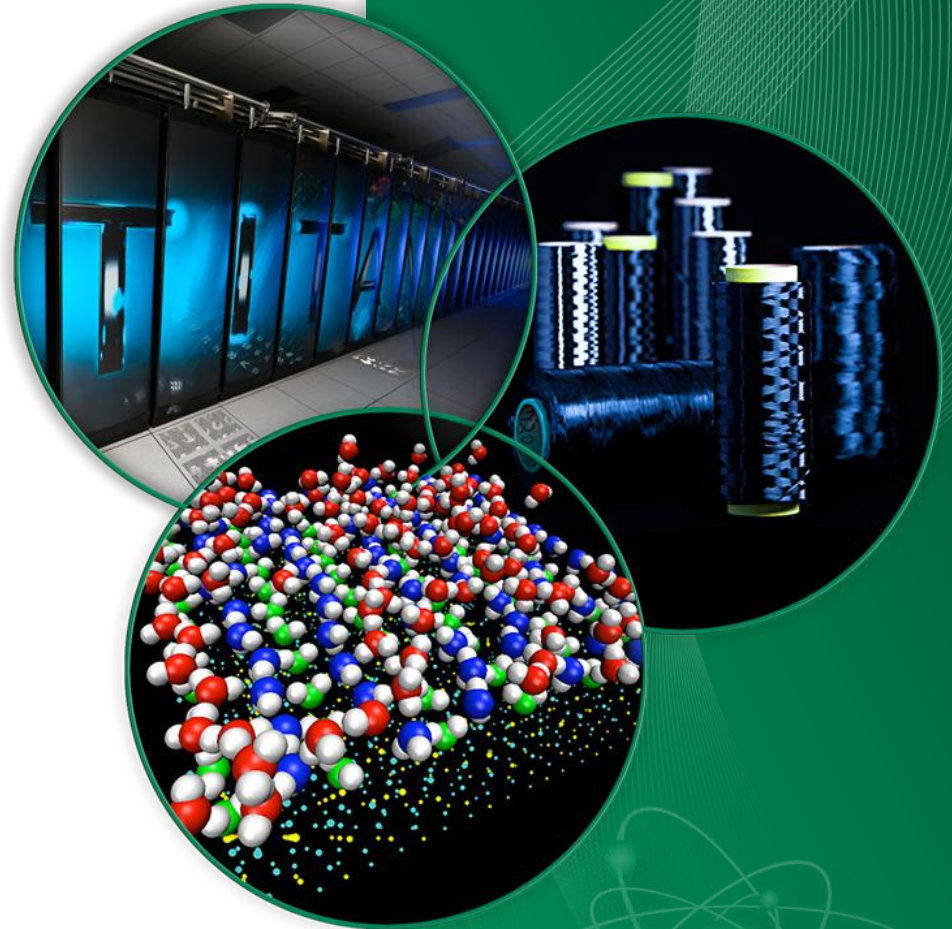


Thoughts on QA for a New ENDF Data Format/Structure

Michael Dunn

WPEC Subgroup 38 Meeting

May 21-22, 2013



Outline

- Mission and Goals
- Needs and Wants
- Roadmap
 - Quality Assurance Plan and Procedures
 - Testing, Testing and Testing
 - Continuous Integration Model and QA
- Needed Resources and Potential Problems/Obstacles

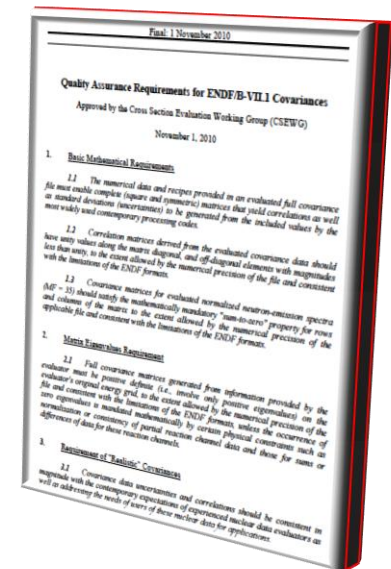
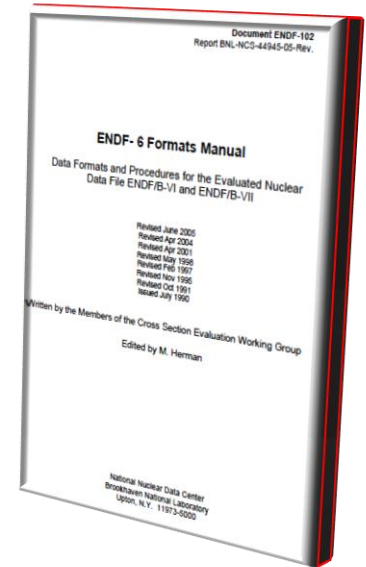


Quality Assurance Plan and Procedures

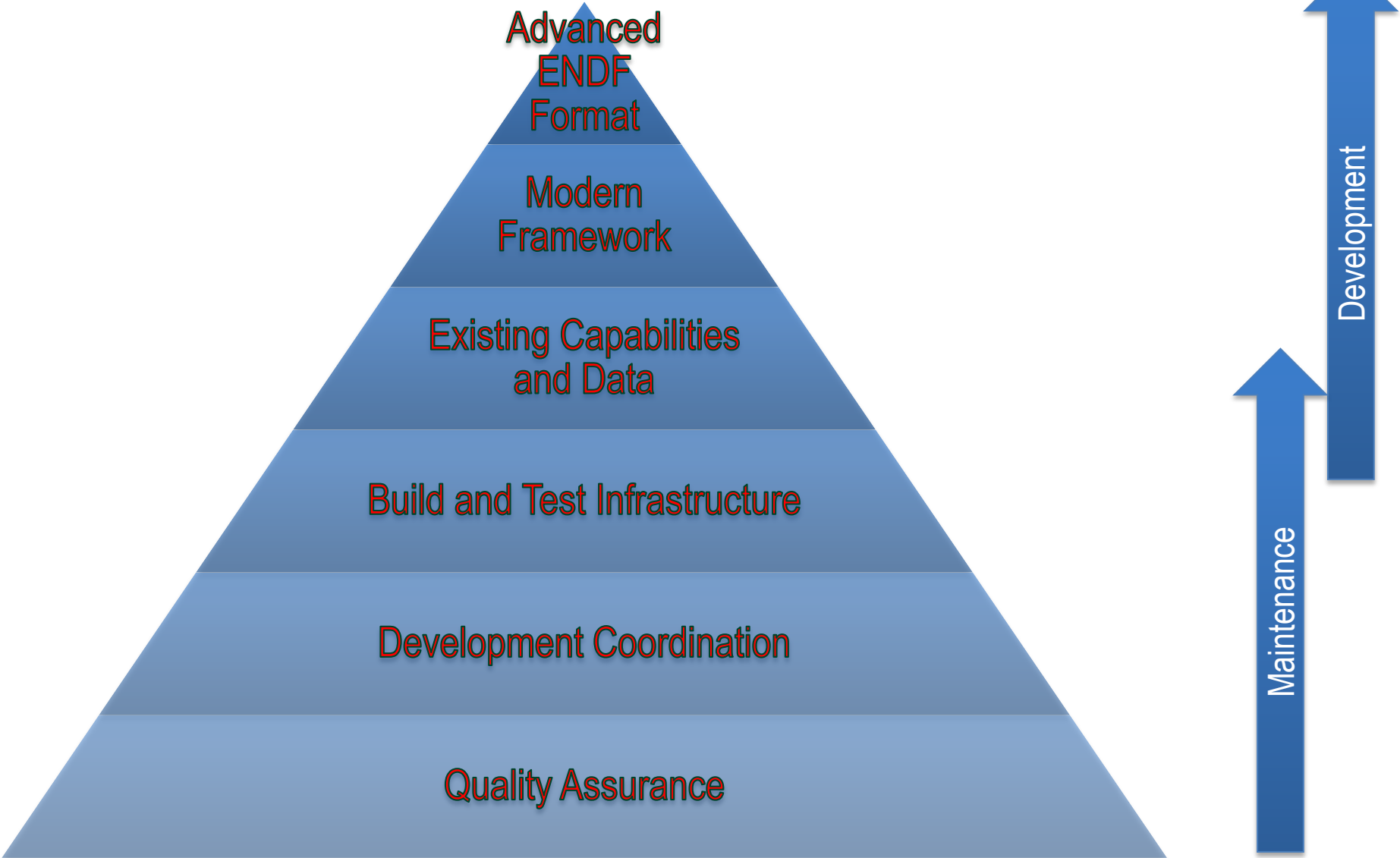
- Mission
 - Develop and implement the quality assurance (QA) infrastructure, which ensures QA requirements are verifiably met and is as low-impact as possible, to support the development, deployment and maintenance of a new, modern international database format/structure.
- Goals (Tasks):
 - Determine 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



ENDF Modernization Roadmap



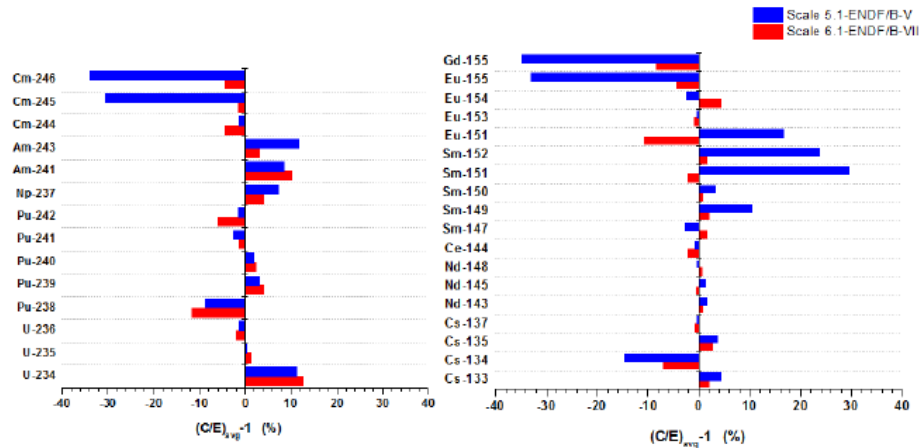
Development Coordination

- Before the QAP can be developed need to define roles and responsibilities for duration of QAP
 - Approval authority for approving and responsible for the QAP (suggestion: SG38 Chair, ENDF Formats Chair, etc.)
 - Records custodian
- ENDF Format Development Team — WPEC SG 38
 - Coordinates overall vision for new ENDF data structure
 - Sets priorities and reviews development progress
 - Meets regularly to coordinate development, deployment, maintenance
- After deployment need to establish long-term maintenance and development plan
 - Use existing ENDF Covariance Committee for long term management of format?
 - Establish on-going WPEC Subgroup (e.g., analogous to HPRL)?
- Team Communication
 - Regular project meetings (SG meetings, CSEWG Formats Meetings, etc.)
 - Development team meetings
 - Wiki pages

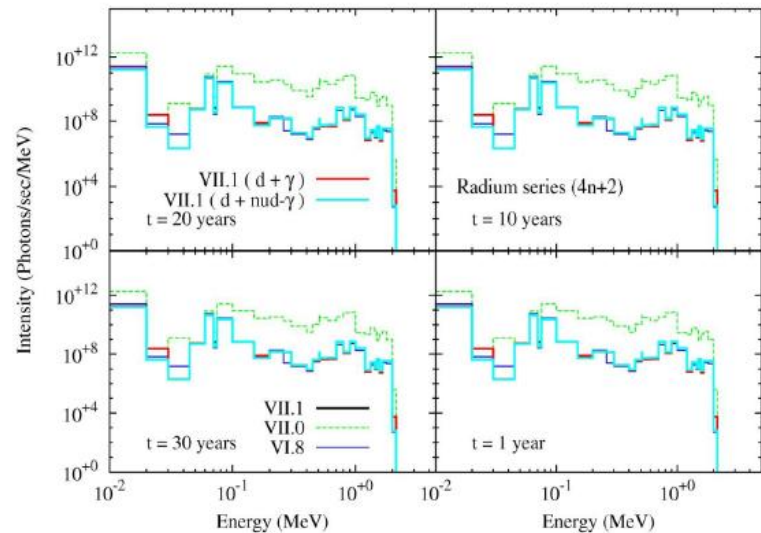
Build and Test Infrastructure

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

Isotopic validation – ENDF/B-V and -VII



Radium decay series (4n+2)



Build and Test Infrastructure

• FogBugz or GForge

- Track QA feature development
- Helpline tickets and email
- Monitor changes to code/data repository

Example from SCALE Development using Fogbugz

FogBugz interface showing a Kanban board with columns for Proposed (6), Approved (0), In Progress (6), In Testing (1), Ready to Ship (1), and Deployed (0). Bug items include 2972: (MLW) CENTRM 2D MoC Option, 2976: (MLW) Sampler, 3080: (BTR) KENO fission density and CE library temperature update for CASL, 3052: (LMPJ) Increase cross name length characters, 3072: (DW) CE library at reactor condi, and 3069: (KB) Updates to Si CASL Bench.

3063

STARBUCS Updates

SCALE: Quality Assurance | Milestone: 6.2 Beta

Assigned to William BJ Marshall (Active)

Charge Number	Sponsor	SCALE Change Log
3530-4T01	NRC SFST	SCALE-2012-011

Technical Reviewer

William BJ Marshall

Functional Specification

STARBUCS functionality has been affected by SCALE updates related to the ORIGEN-S input file format and the SCALE mix limit fix. STARBUCS will be updated to maintain its functionality within SCALE.

Functional Tests

The code functionality will be tested by running the STARBUCS sample problems; the output files will be visually inspected to confirm expected behavior and the results will be compared to the Scale 6.1 results to ensure accuracy. The ENDF/B-V and ENDF/B-VI data are unchanged from 6.1 to dev, just some special nuclides have been renamed for the new mixture limit fix. Since STARBUCS sampling problems use these Scale 6.1 libraries, the changesets are primarily responsible for any significant differences that may be observed for the new calculation results.

Implementation Details

A series of changes were made to implement the new ORIGEN-S input file format and the SCALE mix limit fix and to use proper field length for SCALE_out and _tot files so that the STARBUCS reduced output file contains only the intended output records. Specific changes are as follows:





- (1) use module orglib_io for accessing the ORIGEN-S binary library;
 - (2) use module orgdmp_io to read and write nuclide concentration records to the f71f001 binary file.
 - (3) use modules AmpxLoader, AmpxLibrary, LibraryHeader, and LibraryNuclide to read binary cross-section library header record.
 - (4) update CMakeLists.txt to add the new dependencies.
 - (5) update STARBUCS regression tests to pass within 2 standard deviations; this accommodates platform differences.
- Several STARBUCS subroutines have been modified.

Code repository interface showing a commit history for 'scale'. The history includes entries for 'Merging heads.', 'Updating linker language in tribits for ice, kenova, lava, rade, scale_driv...', 'Updating CELibrary Fortran bindings to fix some issues with gettings and f...', 'Merging Heads.', 'Removed StdCompLib dependency from MipLip. Remov...', 'Fulcrum with addition of CentrmDa...', 'Updated Scalelib's build link list. This resolves linki...', 'The following tests FAILED: 79 -', 'Composition (Failed) 184 - SCLResourceInterface (Failed) 185 - SCLResource (Failed) 187 - SCLResource_M', 'mavric (Failed)', 'mavricUtilities: add capability to mim2wvnp to store just a subset of the groups in the...', 'don't forget to commit', and 'sgmlib: errors in starting a track should be recored as lost particles and not followed f...'.

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 ₃₆	14.1	0	4	477	223.8	2012-03-07T07:48:54 EST	(none)

Build and Test Infrastructure

BNL leading effort to develop ADVANCE – Automated Data Verification and Assurance for Nuclear Calculations Enhancement

Visit <http://www.nndc.bnl.gov/endl/b7.dev/qa/>



General Information:

- ENDF sublib designator: 10
- Revision Number: 592
- Last Modified Revision: 532.592

Build Status:

- Build status: **ALL OK!**
- Build time: 2012-10-24 13:52:00.314153
- Linkfile: neutrons.lib
- Release Notes: neutrons-releaseNotes.pdf

GForge Links:

- Browse SVN
- Browse sublibrary tracker

General Information:

- ENDF MAT designator: 225
- Evaluated date: MAY90
- Evaluation info: LANL
- Evaluation authors: G.Hale, D.Dodder, P.Young
- Natural abundance: 0.000137 +/- 3e-06 %
Check out Wikipedia's entry for helium!

Build Status:

- Build status: **SUCCESS** (submit tracker item)
- Build time: 2012-10-24 13:50:20.874937

GForge Links:

- Browse SVN
- View current revision
- Download current revision

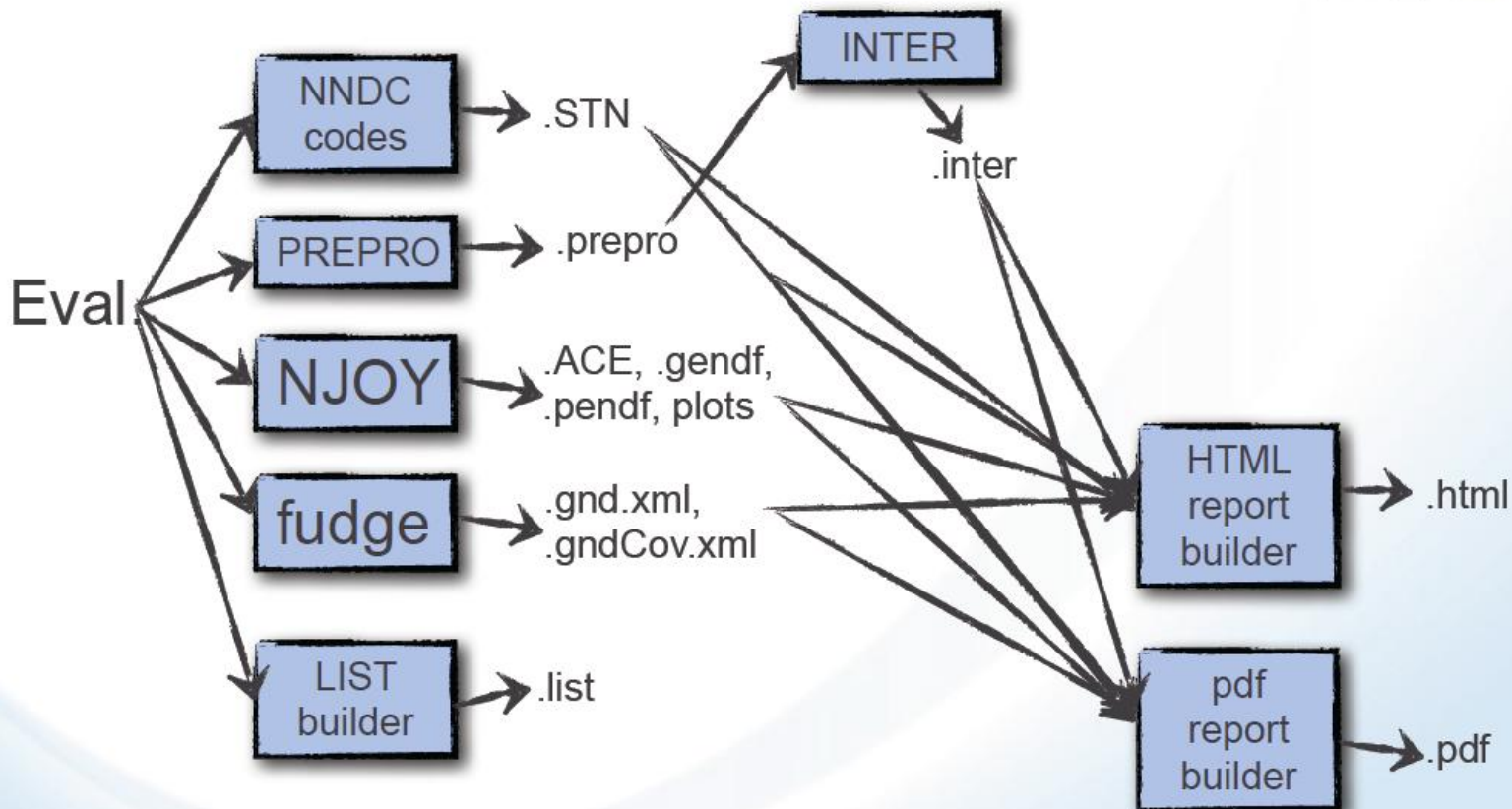
Status	Code	# Tests	# Failures	# Errors	Run time (sec)	Files
✓	STAN	0	0	0	0.033	STN File
✓	STANEF	0	0	0	0.008	
✓	CHECKR	8	0	0	0.012	
✓	FIZCON	8	0	0	0.012	
✓	PSYCHE	16	0	0	0.013	
✓	PREPRO	2	0	0	0.041	prepro File
✓	INTER	1	0	0	0.018	inter File
✓	XXXX.X.X	4	0	4	0.814	Log_gnd.aml File act File, actr.pz File, heat.pz File, heat.chk File, gndff File, radr File, smor.csv File
✓	NJOY99	3	0	0	6.786	

Updated every hour!

Build and Test Infrastructure

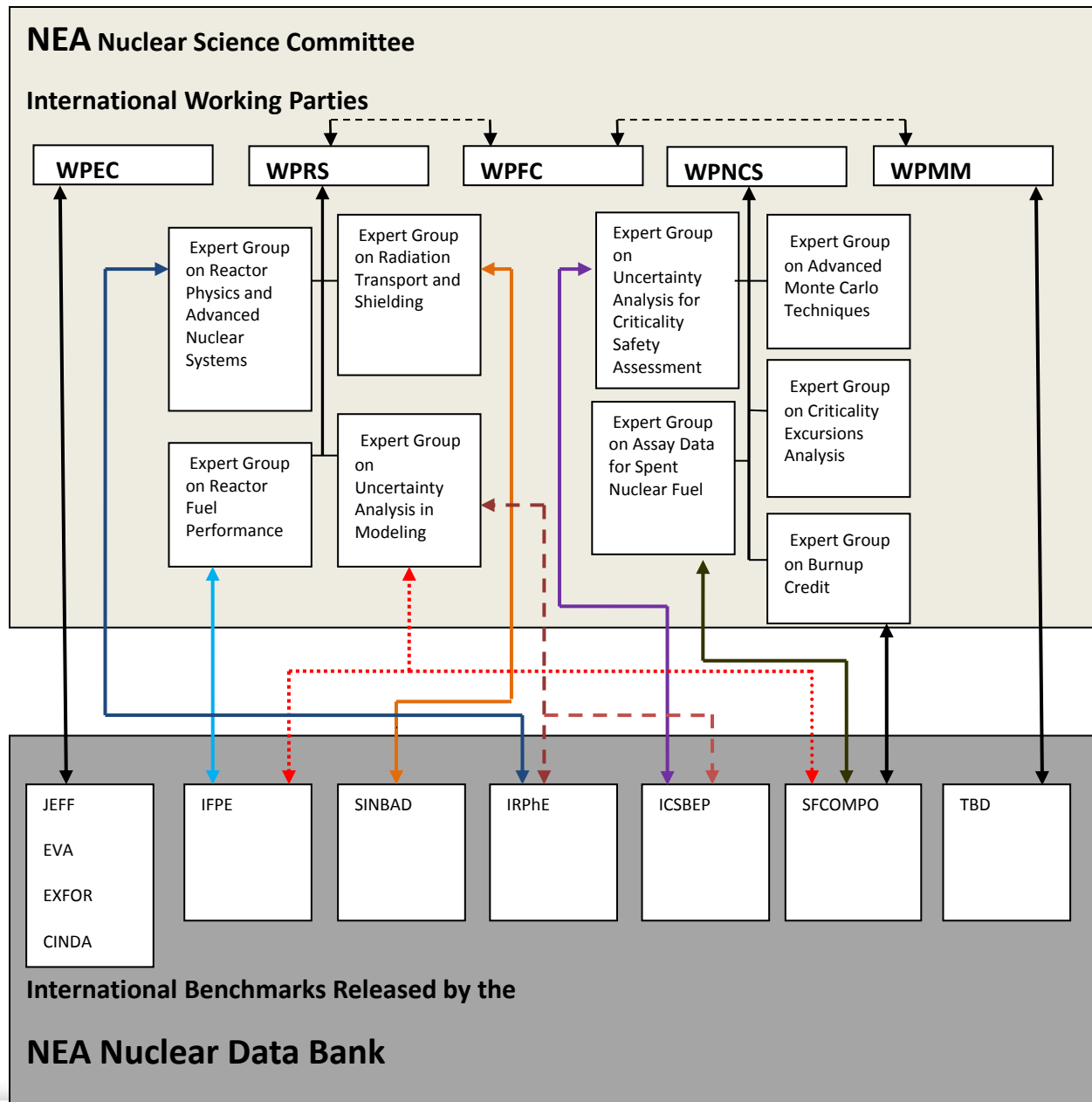
BNL leading effort to develop ADVANCE – Automated Data Verification and Assurance for Nuclear Calculations Enhancement

Current ADVANCE build workflow

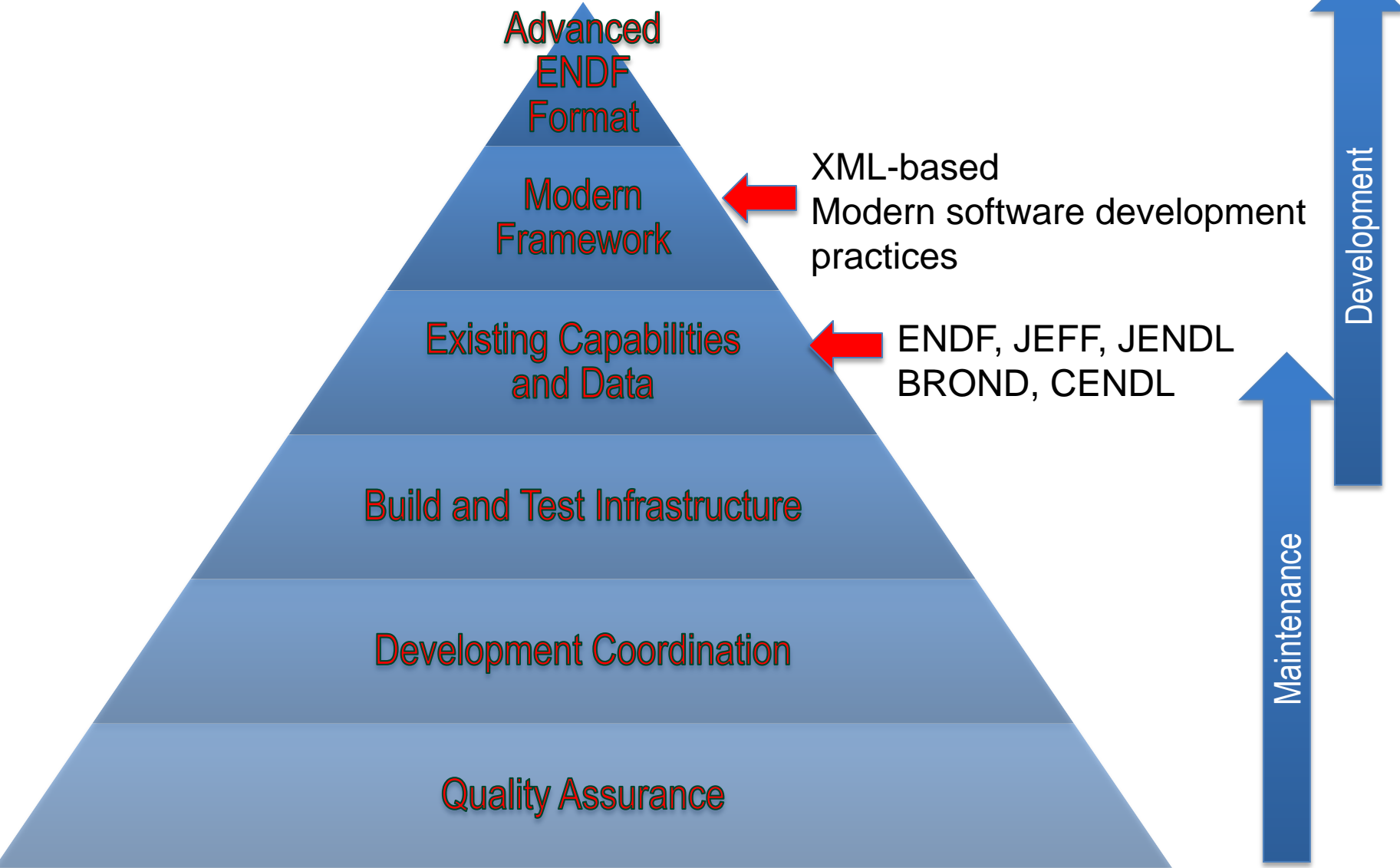


NEA Science Committee and Data Bank

Multiple, international benchmark databases that can be leveraged to support nuclear database V&V



ENDF Modernization Roadmap



Quality Assurance Tasks

- Tasks:
 - Determine the QA requirements – August 2013
 - Develop the QA plan (QAP) with implementing procedures – November 2013
 - Determine and implement the testing requirements to support the QAP implementation and ensure QA – May 2014
 - Develop and deploy the infrastructure needed to provide QA to the nuclear database—continuous integration model – November 2014

Needed Resources and Potential Issues

- Resources
 - Decision points on QAP organization
 - Infrastructure for supporting continuous-integration and testing – Data Centers (staff and computing resources)
- Potential Issues - None