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V&V of MCNP and Data Libraries at Los Alamos

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“Validation and Verification - Tutorial”

ANS Winter Meeting

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LA-UR-12-

Abstract

- **This presentation is part of a tutorial being held at the November 2012 American Nuclear Society Meeting titled "Validation and Verification." In this talk, we describe what V&V is performed on the MCNP code and associated nuclear-data libraries before they are released to users. We indicate why this is of value to end-users, but also indicate why this is not fully sufficient for end-user validation.**

Objective

- **Summarize what Verification and Validation is performed at Los Alamos before releasing production versions of MCNP and data libraries**
  - Why is this of value to end-users?
  - Why is this not sufficient for end-user V&V?

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- and many more …..

Outline

- LANL V&V before production release of a major new nuclear data library for MCNP
- LANL V&V before release of a major new version of MCNP
- Remaining V&V responsibilities of the end user

Keep in mind what Dick McKnight just emphasized:

“Validation always tests Methods, Models, and Data”

LANL V&V Before Production Release of a Major New Nuclear Data Library for MCNP

- **ENDF-6 formatted evaluations need to be processed into a format (ACE) appropriate for MCNP**
  - Los Alamos uses NJOY for this processing
- **The resulting ACE files undergo a series of verification tests**
- **In addition, we perform validation testing of the new data**

Verification Testing of New MCNP Libraries

- ACER module in NJOY performs a number of consistency checks on the ACE file it creates
- Checking scripts are used to analyze the ACE files for potential problems
- Each individual ACE file is used in a simple MCNP verification problem designed to expose issues with the integrity of the file
- Plots for each reaction for each isotope are created and examined for any issues

Objectives of Verification Tests

1. The ACE representations of the data must reproduce the original evaluations as faithfully as possible
2. The ACE files must not contain errors that will cause MCNP to abort
3. The ACE files should not propagate obvious errors in the original evaluations

The verification tests may uncover issues with:

- The original ENDF-6 formatted evaluation
- The NJOY processing
- "Mis-communication" between ENDF-NJOY-MCNP

Examples of Issues Uncovered by Verification Testing

(Examples from ENDF70 neutron library derived from ENDF/B-VII.0)

- **1H: An NJOY update was required to properly process the neutron-induced deuterium production data.**
- **10B: a leading non-zero threshold photon production cross section value was found for the isotope (MCNP MT=103004). That value was changed to zero and the total photon production cross section at that energy was decremented accordingly.**
- ***45Sc: The cross section for nonelastic photon* production (MF=13, MT=3) did not have a zero point at the threshold; one was inserted. Additionally, the evaluation had the incorrect reference frame specified for angular distributions of (n,2n), (n,n*)a, (n,n*)p, and (n,n*c). We made changes to the evaluation and re-processed.**

Examples of Issues Uncovered by Verification Testing

- ***89Y: Negative cross sections for MT=91 from 1.7 to* 4.5 MeV were found. These data were modified to be the difference between MT 4 (total inelastic) and the sum of MT's 51-90 (partial inelastic).**
- **96Zr and 97Mo: NJOY's CONSIS module identified errors in several MF=6 Law=44 "r" values that were subsequently changed from 0.999999e+1 to 0.999999e+0.**
- **153Eu: Negative probability density functions were found at several incident energies for MF=6, MT=91. The negative pdf's were set to 0.0 and the distributions were renormalized.**
- **242Am (ground): The angular distribution for fission was missing, so we inserted an isotropic MF=4, MT=18 section.**

Examples of Issues Uncovered by Verification Testing

- 242mAm: The inelastic cross sections (MT 4, 51, 52, 53, and 54) contained values of zero between 50 and 65 keV, whereas values above and below this energy range were non-zero. The cross sections below 100 keV were smoothed out by the evaluator.
- Unresolved resonance data for several minor isotopes could not be successfully processed into ACE probability-table format.
- Energy-balance problems were identified and noted for several evaluations.
- U-233: There was an error in the exponent for the delayed- neutron yields for U-233 above 9 MeV, which should be e-3 instead of e-2.
- Desired improvements in fidelity of specified interpolation of secondary neutron data for actinides were documented.

These issues (including fixes for several evaluations) were communicated to CSEWG

Validation Testing of New MCNP Data Libraries

(Examples from MCNP neutron library derived from ENDF/B-VII.1)

- **A variety of ICSBEP benchmark assemblies have been calculated with ENDF/B-VII.1 data and MCNP5**
- **Time limitations in this talk prevent detailed discussion of results**
- **See sample results from Dick McKnight's presentation**
- **See paper presented by Skip Kahler at this meeting: "LANL Evaluation and Data Testing Support for ENDF/B-VII.1," p. 683 of Transactions.**
- **See large ENDF/B-VII.1 data testing report published in December 2011 Nuclear Data Sheets: A.C. Kahler *et al*, Nuclear Data Sheets, <u>112</u>, Issue 12, (2011) 2997–3036.**

Verification Testing of New Version of MCNP

- **See papers presented at this meeting:**
  - Brian Kiedrowski : “Verification of MCNP5-1.60 and MCNP6-Beta2 for Criticality Safety Applications,” page 605 of Transactions
  - Forrest Brown: “MCNP Monte Carlo Progress – Nuclear Criticality Safety,” page 694 of Transactions
- **Current emphasis – transition from MCNP5 to MCNP6.**
  - Substantial expansion of code functionality with impacts on core MCNP transport routines
  - Objective is to ensure that criticality results are not negatively impacted

MCNP: Nightly Regression Tests and V&V Suites

- **Continuous Test System for MCNP6**
  - 3 platforms - Linux 32, Linux 64, Windows 64
  - 5 compilers - Intel 10+11, PGI 7, Pathscale 3, gfortran
  - Serial, mpi, omp, mpi+omp
  - Array bounds checking
  - 875 problem input files
  - Total: 10,000 runs each night
- **MCNP V&V Suites**
  - Physics-based V&V
  - Compare to experiment or exact analytic results
  - Part of MCNP permanent code repository & RSICC distribution
  - Automated - easy to run & collect results, compare to experiments

Recent and Current MCNP V&V Studies

MCNP5-1.51 – 2008

MCNP5-1.60 – 2010

MCNP6-Beta-2 – 2012

- **For a given Criticality V&V Suite:**

1. Compare **MCNP versions** using:
   - ENDF/B-VII.0 data + Intel-10.1 Fortran-90
2. Compare **F90 compilers** using:
   - MCNP + ENDF/B-VII.0 data
3. Compare ENDF/B-VII.0 vs ENDF/B-VII.1 **data** using:
   - MCNP + Intel-11.1 F90

V&V Testing for MCNP5-1.60 (from LA-UR-11-06130)

MCNP5-1.60 Release (3)

mcnp Monte Carlo Codes XCP-3, LANL

- **Testing + V&V Suites**

REGRESSION	- 66 installation & regression test problems
VALIDATION_CRITICALITY	- 31 ICSBEP Handbook cases
VERIFICATION_KEFF	- 75 analytic problems, exact results
VALIDATION_SHIELDING	- 19 shielding/dose problems vs experiment
KOBAYASHI [new]	- void & duct streaming, point detectors
POINT_KINETICS [new]	- adjoint weighted Rossi-α, β_{eff}, Λ_{eff}

- **Computers**
  - Mac / Linux / Windows, 32 / 64 bit
  - Sequential, threads, MPI, threads+MPI
  - Over 5,000 hr computer time
  - 2 students full-time + 2.5 staff part-time for 3 months

- **Criticality calculations**
  - Tested with ENDF/B-VI & ENDF/B-VII.0
  - All results should match previous versions of MCNP5

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V&V Testing for MCNP5-1.60 (from LA-UR-11-06130)

MCNP5-1.60 Release (4)

Monte Carlo Codes
XCP-3, LANL

MCNP Criticality Validation Suite, Results on Mac OS X for ENDF/B-VII.0

	Experiment	MCNP5-1.51	MCNP5-1.60
U233 Benchmarks			
JEZ233	1.0000 (10)	0.9989 (6)	0.9989 (6)
FLAT23	1.0000 (14)	0.9990 (7)	0.9990 (7)
UMF5C2	1.0000 (30)	0.9931 (6)	0.9931 (6)
FLSTF1	1.0000 (83)	0.9830 (11)	0.9830 (11)
SB25	1.0000 (24)	1.0053 (10)	1.0053 (10)
ORNL11	1.0006 (29)	1.0018 (4)	1.0018 (4)
HEU Benchmarks			
GODIVA	1.0000 (10)	0.9995 (6)	0.9995 (6)
TT2C11	1.0000 (38)	1.0018 (8)	1.0018 (8)
FLAT25	1.0000 (30)	1.0034 (7)	1.0034 (7)
GODIVR	0.9985 (11)	0.9990 (7)	0.9990 (7)
UH3C6	1.0000 (47)	0.9950 (8)	0.9950 (8)
ZEUS2	0.9997 (8)	0.9974 (7)	0.9974 (7)
SB5RN3	1.0015 (28)	0.9985 (13)	0.9985 (13)
ORNL10	1.0015 (26)	0.9993 (4)	0.9993 (4)

	Experiment	MCNP5-1.51	MCNP5-1.60
IEU Benchmarks			
IMF03	1.0000 (17)	1.0029 (6)	1.0029 (6)
BIGTEN	0.9948 (13)	0.9945 (5)	0.9945 (5)
IMF04	1.0000 (30)	1.0067 (6)	1.0067 (6)
ZEBR8H	1.0300 (25)	1.0195 (6)	1.0195 (6)
ICT2C3	1.0017 (44)	1.0037 (7)	1.0037 (7)
STACY36	0.9988 (13)	0.9994 (6)	0.9994 (6)
LEU Benchmarks			
BAWXI2	1.0007 (12)	1.0013 (7)	1.0013 (7)
LST2C2	1.0024 (37)	0.9940 (6)	0.9940 (6)
Pu Benchmarks			
JEZPU	1.0000 (20)	1.0002 (6)	1.0002 (6)
JEZ240	1.0000 (20)	1.0002 (6)	1.0002 (6)
PUBTNS	1.0000 (30)	0.9996 (6)	0.9996 (6)
FLATPU	1.0000 (30)	1.0005 (7)	1.0005 (7)
THOR	1.0000 (6)	0.9980 (7)	0.9980 (7)
PUSH2O	1.0000 (10)	1.0012 (7)	1.0012 (7)
HISHPG	1.0000 (110)	1 0122 (5)	1.0122 (5)
PNL2	1.0000 (65)	1.0046 (9)	1.0046 (9)
PNL33	1.0024 (21)	1.0065 (7)	1.0065 (7)

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MCNP6 Verification / Validation Suites

- **MCNP V&V Suites**

VALIDATION_CRITICALITY	31 ICSBEP experiment benchmarks
VALIDATION_CRIT_EXPANDED	119 ICSBEP experiments
CRIT_LANL_SBCS	194 ICSBEP experiments, from LANL crit-safety group
VERIFICATION_KEFF	75 analytic benchmarks, exact solutions
VALIDATION_ROSSI_ALPHA	Rossi alpha vs experiment
VALIDATION_ACODE	static-alpha eigenvalue benchmarks
POINT_KINETICS	reactor kinetics parameters
KOBAYASHI	void & duct streaming, with point detectors, exact solutions
VALIDATION_SHIELDING	19 shielding/dose experiments
REGRESSION	66 code test problems
many others for MCNP6	electrons, protons, muons, high-energy physics, delayed particles, magnetic fields, point detectors, MCNP6/Partisn weight window generator, unstructured mesh & ABAQUS linkage, photons, pulse height tallies, string theory models

MCNP6 Verification Results: VALIDATION_CRITICALITY Suite – Codes & Compilers

31 ICSBEP experiment benchmarks, ENDF/B-VII.0 nuclear data

- **MCNP5-1.51, MCNP5-1.60, MCNP6-Beta-2**
  - Intel-10.1 Fortran-90 compiler for **all 3**: **All results match exactly**
- **MCNP5-1.60, MCNP6-Beta-2**
  - Intel 10.1 F90 for **both**: **All results match exactly**
  - Intel 11.1 F90 for **both**: **All results match exactly**
  - Intel 12.0 F90 for **both**: **All results match exactly**
  - Intel 11.1 vs 12.0 F90 for **both**: **All results match exactly**
  - Intel 10.1 vs 11.1/12.0 F90 for **both**:
    - **For 27 problems, results match exactly**
    - **For 4 problems, results differ due to roundoff, match within statistics**
- **Conclusions**
  - **Using the same F90 compiler,
MCNP5-1.51, MCNP5-1.60, MCNP6-Beta-2 all match results exactly**
  - **Switching from Intel-10 to Intel-11/12 introduces some small computer roundoff differences – compiler issue, not code or results**

MCNP6 Verification Results: Comparisons Using Other Criticality Suites

- **VALIDATION_CRIT_EXPANDED**
  - 119 ICSBEP experiments
  - ENDF/B-VII.0 data
  - **MCNP5-1.60** vs **MCNP6-Beta-2**, with Intel-12.0 F90
    - **For 116 problems, results match exactly**
    - **For 3 problems, results differ due to roundoff, match within statistics**
- **CRIT_LANL_SBCS**
  - From LANL SB-CS Group, criticality-safety validation suite
  - 194 ICSBEP experiments
  - ENDF/B-**VI** data
  - **MCNP5-1.60** vs **MCNP6-Beta-2**, with Intel-10.1 F90
    - **For 192 problems, results match exactly**
    - **For 2 problems, results differ due to roundoff, match within statistics**
  - **MCNP5-1.60** (2010, Intel-10) vs **MCNP5-1.25** (~2003, Intel-9)
    - **For 144 problems, results match**
    - **For 50 problems, results differ due to roundoff, match within statistics**

User Responsibilities

- **Previous material should convince criticality-safety users that when they receive a production version of MCNP / MCNP Data Libraries, they should be extremely confident in the rigor of the testing, verification, and validation processes that the code and data have undergone.**
- **BUT**
- **Los Alamos developers cannot validate the code and data for YOUR application – this remains YOUR responsibility**
  - Other presentations during this tutorial provide guidance for you to do so
  - You should also pay attention to “Best Practices” guidance from Los Alamos developers
    - “Validation always tests Methods, ***Models***, and Data”

Best-Practice Guidance for Criticality Problems

- **See extensive documentation available at http://mcnp.lanl.gov**
- **Best Practices - Convergence, Bias, Statistics**
  - F.B. Brown, “A Review of Best Practices for Monte Carlo Criticality Calculations”, ANS NCSD-2009, Richland, WA, Sept 13-17 paper LA-UR-09-03136, presentation LA-UR-09-05623 (2009).
  - F.B. Brown, "A Review of Monte Carlo Criticality Calculations - Convergence, Bias, Statistics", M&C-2009, Saratoga Springs, NY, May, 2009, paper LA-UR-08-06558, presentation LA-UR-09-02377 (2009).
  - F.B. Brown, “‘K-Effective Of The World’ And Other Concerns For Monte Carlo Eigenvalue Calculations”, SNA+MC-2010, Tokyo, Oct 17-2 paper LA-UR-10-05548, presentation LA-UR-10-06874 (2010)
  - F.B. Brown, “Revisiting the ‘K-effective of the World’ Problem”, Trans. Am. Nuc. Soc, 102, June 2010, LA-UR-10-00189 (2010).
  - F.B. Brown, "Monte Carlo Eigenvalue Calculations", LA-UR-06-7094 (2006).
  - B.C. Kiedrowski, F.B. Brown, "Difficulties Computing k in Non-Symmetric, Multi-Region Systems with Loose, Asymmetric Coupling," International Conference on Nuclear Criticality, Edinburgh, Scotland, 19-22 September 2011, LA-UR-11-04541 (2011).

Best-Practice Guidance for Criticality Problems (Directly from LA-UR-09-05623)

- **To avoid bias in Keff & tally distributions, use 10K or more neutrons/cycle**
- **Always check convergence of both Keff & Hsrc**
- **Take advantage of problem symmetry, if possible**
- **Use a good initial source guess, uniform in fissionable regions**
- **Run at least a few hundred active cycles to allow codes adequate information to compute statistics**
- **Be aware that statistics on tallies from codes are underestimated, possibly make multiple independent runs**

How Should Users Select Cross-Section Tables?

- **Various strategies:**
  - Just use defaults
  - Always use the latest
  - Use tables / libraries validated for you application
- **Things to consider:**
  - Specific application – what's important?
    - Neutron-induced photon production?
  - Detail provided in table (check table length and number of energies)
  - Temperature
  - Consider swapping out tables to check sensitivity
  - Detailed documentation associated with evaluation source, MCNP library creation, validation studies, etc.
- **Also make sure that MCNP physics options (e.g., prompt / delayed nubar / spectra, temperature, probability tables, thermal S(α,β) tables, etc.) are appropriate for your problem**

Summary

- **Los Alamos invests substantial effort to ensure that production releases of MCNP and MCNP data libraries have undergone rigorous testing, verification, and validation**
- **This work is necessary, but not sufficient**
- **Criticality-safety end users have final responsibility for validation of specific applications**
  - Being smart code and data users helps to fulfill that responsibility