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LANL-SNL Collaboration on NCS Validation

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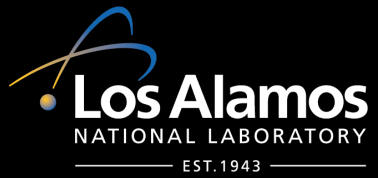

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[1] LANL, [2] SNL

Abstract

LANL-SNL Collaboration on NCS Validation

Forrest Brown[1], John Miller[2], Shawn Henderson[2], Michael Rising[1], Jennifer Alwin[1]

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During 2016, nuclear criticality safety (NCS) practitioners from SNL and code developers from LANL collaborated in several areas of interest to the DOE/NNSA Nuclear Criticality Safety Program (NCSP). This collaboration involved

- Testing of the preliminary release of the MCNP6-Whisper methodology, with feedback to the developers,
- Sharing of the benchmark catalogs
- Comparison and analysis of benchmarks common to both catalogs,
- Investigation of the impact of the different benchmark catalogs on sensitivity-uncertainty based NCS validation results from MCNP6-Whisper,
- Investigation of the impact of randomized selections from the benchmark catalog on sensitivity-uncertainty based validation results from MCNP6-Whisper.
- Investigation of the use of MCNP6-Whisper in selecting benchmarks for use in NCS validation for unique, nonstandard, legacy fuel applications.

This talk summarizes the collaboration work and initial results. It must be noted that the results described herein are preliminary and need further research and detailed analysis. However, the initial results are very interesting, and it is important to share them with the NCSP community.

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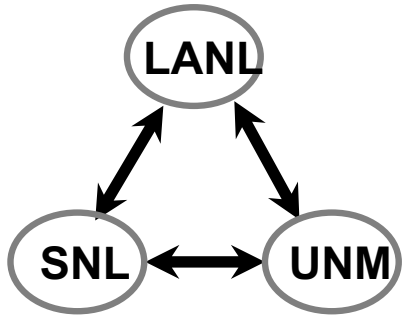
Background

- **2015**
  - **Miller: issued SNL report on NCS validation**
  - **Brown: requested copies of benchmarks**
  - **Brown: UNM Professor, teaching Monte Carlo class**
  - **Henderson: UNM student in MC class, intern at SNL**



- **2016**
  - **Miller**
    - Challenged by NCS validation for old U-Gd fuel
    - Interested in using Whisper to identify proper benchmark catalog
  - **Henderson**
    - Changed SNL internship to NCS with Miller
    - Graduated from UNM Nuclear Engineering
    - Summer work at SNL, Whisper applications, with Miller/Brown
    - First use of Whisper outside of LANL
    - Now NCS staff

Collaboration Activities

- Test preliminary release of the MCNP6-Whisper, with feedback to the developers
- Share benchmark catalogs (1101 LANL cases, 866 SNL cases)
- Compare 357 benchmarks common to both catalogs
- Investigate the impact of the different benchmark catalogs on sensitivity-uncertainty based NCS validation results from MCNP6-Whisper
- Investigate the impact of randomized selections from the benchmark catalog on sensitivity-uncertainty based validation results from MCNP6-Whisper
- Investigate the use of MCNP6-Whisper in selecting benchmarks for use in NCS validation for unique, nonstandard, legacy fuel applications

MCNP6-Whisper Testing

- **Whisper**
  - **Statistical analysis code to determine baseline USLs**
  - **Uses sensitivity profiles from continuous-energy MCNP6**
  - **Uses covariance data for nuclear cross-sections**

    ① **Automated, physics-based selection of benchmarks that are neutronically similar to the application, ranked & weighted**

    ② **Bias + bias uncertainty from Extreme Value Theory**

    ③ **Margin for nuclear data uncertainty estimated by GLLS method**

- **SNL testing**
  - **MCNP6.1.1, Whisper-1.1, ENDF/B-VII.1 data**
  - **Whisper-1.1**
    - Upgrade from original Whisper – portable to Mac, Windows, Linux
  - **First non-LANL, independent testing, on different computers**
    - Henderson – very capable, but new to NCS
    - No trouble installing & applying to SNL applications
    - Provided valuable feedback to LANL on details & a few minor fixes
    - Lessons-learned were addressed for upcoming Whisper release

Sharing Benchmark Catalogs

- **LANL catalog of 1101 ICSBEP problems**
  - **1086 from 2014 validation for PF4**
  - **15 new cases from LANL NCS, some corrections to previous problems**

- **SNL catalog of 866 ICSBEP problems**
  - **265 from 2015 validation report**
  - **601 from Miller & others, currently under review**
  - **SNL updated all benchmarks to current recommendations:**
    - Use isotopes (not elements)
    - ENDF/B-VII.1 cross-section data, with continuous S(α,β)
    - Follow "Best Practices"
      - Shannon entropy checks on convergence
      - Use at least 10,000 neutrons/cycle & at least 100 active cycles

Comparison of Benchmark Catalogs (1)

- 357 cases were common to the LANL & SNL benchmark catalogs
- Is there any evidence of "analyst bias" or "site bias" ?
  - Different analysts at different sites set up the 357 common benchmarks independently based on ICSBEP specifications
  - The benchmarks were run using the same code, the same nuclear data, and the same Monte Carlo "best practices"
  - Any bias determined from the 357 common cases would suggest differences due to analyst modeling procedures

Table 1. Comparison of common benchmarks

	Bias ± Std.Dev
357 LANL cases	0.00175 ± 0.00024
357 SNL cases	0.00179 ± 0.00021
Ave. SNL-LANL	0.00004 ± 0.00010

  - No apparent evidence of "analyst bias", but still investigating

Comparison of Benchmark Catalogs (2)

- **Comparison of computed k_{eff} for the 357 common benchmarks**
  - **339 agreed within 0.001 Δk**

Table 2. Distribution of differences in common cases

range for $\lvert k_{SNL}-k_{LANL}\rvert$	Number of cases
< 0.001	339
0.001 – 0.002	8
0.002 – 0.003	3
0.003 – 0.004	1
0.004 – 0.005	1
> 0.005	5

  - **The 18 cases with differences greater than 0.001 Δk are being reviewed:**
    - A few differ due to including impurities, or not
    - A few differ due to simplified vs detailed geomtetry
    - A few may have errors
    - Detailed review is still in progress
  - **This type of review & QA is new & valuable to both LANL & SNL**

Impact of Benchmark Catalogs on USL Results

- **For a few applications, baseline USLs were computed using MCNP6-Whisper using different benchmark catalogs**
  - **SNL catalog only (866 cases)**
  - **LANL catalog only (1101 cases)**
  - **SNL catalog, with non-duplicate additions from LANL (1610 cases)**
  - **LANL catalog, with non-duplicate additions from SNL (1610 cases)**
- **For 1 specific SNL application**

Table 3. Catalog USL calculations

Benchmark Catalog	Highest C_k	Bias+Bias Uncertainty	Calculated USL
SNL	0.9902	0.01624	0.97747
LANL	0.9924	0.01715	0.97656
SNL+LANL	0.9924	0.01691	0.97680
LANL+SNL	0.9924	0.01691	0.97680

  - **Results agree very well, but of course further studies are needed**

Impact of Randomized Benchmark Catalogs

- **Seven applications related to the LANL PF4 Facility were chosen**
  - **Each was run with Whisper 25 times using the LANL catalog**
  - **For each of the 25 runs for a case, 50% of the benchmark cases were selected randomly and excluded from the Whisper calculations**
  - **The minimum, average, and maximum of the 25 USLs for each case are:**

Table 4. Whisper results for 25 repetitions using random 50% of benchmark catalog

Application	Whisper baseline USL		
	Min	Ave	Max
1 - Pu cylinder, H/D=0.5	0.978	0.979	0.981
2 - Pu cylinder, H/D=3.0	0.977	0.979	0.980
3 - Pu annulus, H/D=1.0, IR=0.001	0.978	0.979	0.981
4 - Pu annulus, H/D=1.0, IR=0.5	0.978	0.979	0.981
5 - Pu – NaCl sphere, 1" water refl	0.975	0.977	0.978
6 - Pu sphere, 0.01 cm Ta reflector	0.978	0.979	0.981
7 - Pu sphere, 5.0 cm Ta reflector	0.924	0.929	0.933

- All cases used 4500 g of Pu-239
- Cases 1-4 used 2.54 cm radial water reflector
- Cases 3-4 used water in center of annulus
- Cases 6-7 used spherical Pu with Ta reflector

  - **Cases 1-6 agreed well, insensitive to variations in benchmark catalog**
  - **Case 7 more sensitive, but reflects the lack of Ta-reflected benchmarks**
  - **Despite variations in benchmark catalog, Whisper selects best matches**

Benchmark Selection for Nonstandard Applications

- **One of the drivers for the collaboration**

  - **SNL needed to evaluate some applications involving legacy uranium-gadolinium fuel**

    - Was the recent 2015 SNL validation applicable?
    - Initial MCNP-Whisper analysis indicated NO
      - Traditional SNL validation did not adequately cover neutronics of the U-Gd fuel
      - Whisper correlation coefficients with traditional validation catalog were low

  - **SNL added 77 additional ICSBEP benchmarks containing Gd to their catalog**

    - Whisper was happy – good correlations found between U-Gd fuel applications & expanded benchmark catalog

    - This effort will be written-up & reported separately, since it provides valuable “lessons-learned”

Sensitivity-uncertainty tools can provide valuable quantitative evidence regarding the adequacy of the benchmark catalog for validation

Summary

- **Benefits of the collaboration**
  - Additional QA, testing, and checking of the benchmark catalogs
  - Identification of specific benchmarks that warrant further detailed review.
  - Combined effort eases the task of expanding the benchmark catalogs for use in NCS validation.
  - Feedback from independent, external testing of a new software package (Whisper) strengthens the usability and SQA. Lessons-learned can be dealt with prior to the official public release of the software.
  - Initial comparisons suggest that no apparent “analyst bias” is present between the NCS validation work at the respective sites.
  - Different sets of benchmarks in the catalogs have only small effects on the baseline USLs determined by the MCNP6-Whisper methodology

Future Work

- **The LANL-SNL collaboration work to date has benefitted both sites, and both are interested in continuing this work.**
- **The preliminary results to date suggest a number of worthy areas for additional collaboration:**
  - **Expand both benchmark catalogs**
  - **Perform more real-world application testing on the use of MCNP6-Whisper based NCS validation, including comparisons with traditional NCS validation methods**
  - **Perform further detailed analysis using the different benchmark catalogs, to thoroughly investigate the notion of "analyst bias"**
  - **Explore the use of the MCNP6-Whisper methodology for applications where there are not a sufficient number of ICSBEP benchmarks available**

Questions ?