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LANL-SNL Collaboration on NCS Validation

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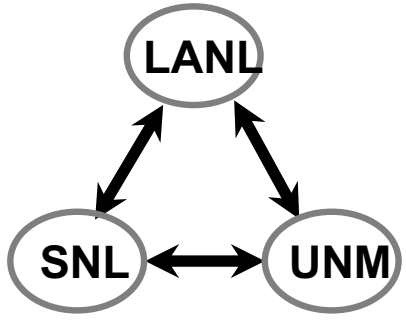
Background

- **2015**
  - **Miller: 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**

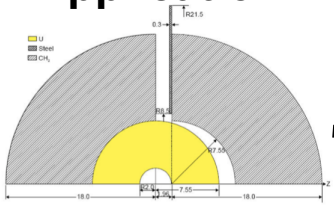


- **2016**
  - **Miller**
    - Challenged by NCS validation for old U-Gd fuel
    - Interested in using Whisper to identify proper benchmark catalog
  - **Henderson**
    - Changed SNL internship to NCS with Miller
    - Graduated from UNM Nuclear Engineering
    - Summer work at SNL, Whisper applications,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

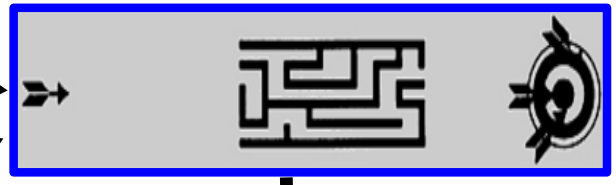
MCNP6 & Whisper – Overview

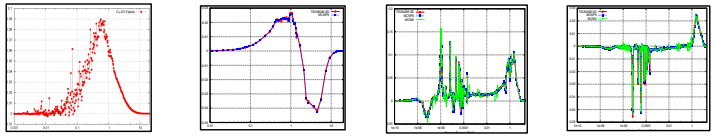
From LA-UR-16-23757

Application



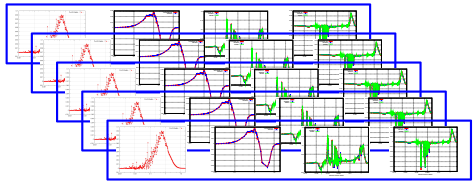
ACE Cross-section Data





ACE Cross-section Covariance Data

SU-based Analysis



Catalog of sensitivity profiles for 1100+ experiments

USL
Upper Subcritical Limit for NCS analysis

MCNP6

Monte Carlo Criticality Calculation

Application Sensitivity Profile

Whisper

Pattern matching – application sensitivity profile vs catalog

Select similar experiments

Statistical analysis to determine bias & uncertainty & MOS

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 LANL & SNL & NCSP

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	Whisper Baseline-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**

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Questions ?