MCNP® Status and Modernization

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Monte Carlo Methods, Codes, & Applications (XCP-3)
X Computational Physics Division

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NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

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Abstract

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Monte Carlo Methods, Codes, & Applications, LANL

The DOE-NNSA Nuclear Criticality Safety Program (NCSP) supports research, development, maintenance, verification and validation, user support, and training for the MCNP Monte Carlo code for nuclear criticality safety (NCS) customers within DOE-NNSA.

The MCNP Monte Carlo code has been used for high-fidelity analyses of criticality safety problems since the 1970s. This talk summarizes MCNP progress during FY 2018 and early FY 2019. Activities and accomplishments are summarized in five major areas:

- MCNP6 & Whisper status
- Verification and validation testing
- User support, training & education
- R&D work in progress
- MCNP code modernization

Work supported by: US DOE-NNSA Nuclear Criticality Safety Program

MCNP® Status and Modernization

US DOE-NNSA Nuclear Criticality Safety Program –

What have we done for you lately (FY 2018, FY 2019) ?

- **Overview of LANL Analytical Methods Work for NCSP**
- **MCNP6 & Whisper Status**
- **Verification / Validation**
- **User Support, Training & Education**
- **R&D Work in Progress**
  - Automated Acceleration & Convergence Testing*
  - Impact of Outliers on NCS Validation and USLs*
  - Machine Learning Methods using Nuclear Data Sensitivities*
  - Correlated Fission Multiplicity in Critical & Subcritical Simulations
  - Region-wise Sensitivities for NCS Validation
- **MCNP Code Modernization**

*** = separate presentations at the 2019 NCSP TPR**

Overview of LANL Analytical Methods Work for NCSP

MCNP6 & Whisper Code Development

- New features & friendly testing
- Maintenance & bug fixes
- External releases
- Code modernization

Research & Development Projects

- Methods & Algorithms
- Parallel Performance
- Physics Options
- USLs & Validation

Verification & Validation

- Automated V&V testing
- New/updated validation suite development & testing
- Daily/nightly behavioral testing

User Support, Training & Education

- Monte Carlo Classes at UNM
- MCNP Criticality Training
- Whisper S/U Training
- Reference collection, web site, forum, etc.

MCNP6 & Whisper Status

MCNP6 & Whisper Status (1)

- **MCNP releases by RSICC**

MCNP6.1 – 2013, production version
MCNP6.1.1 – 2014, same criticality, faster, beta features for DHS
MCNP6.2 – 2018, with Whisper code & benchmarks & about 2x faster than MCNP6.1

Nuclear Data – ENDF/B-VII.1 data, updates, & older data
Reference Collection – 700^{+} technical reports
V&V Test Collection – 1500^{+} test problems

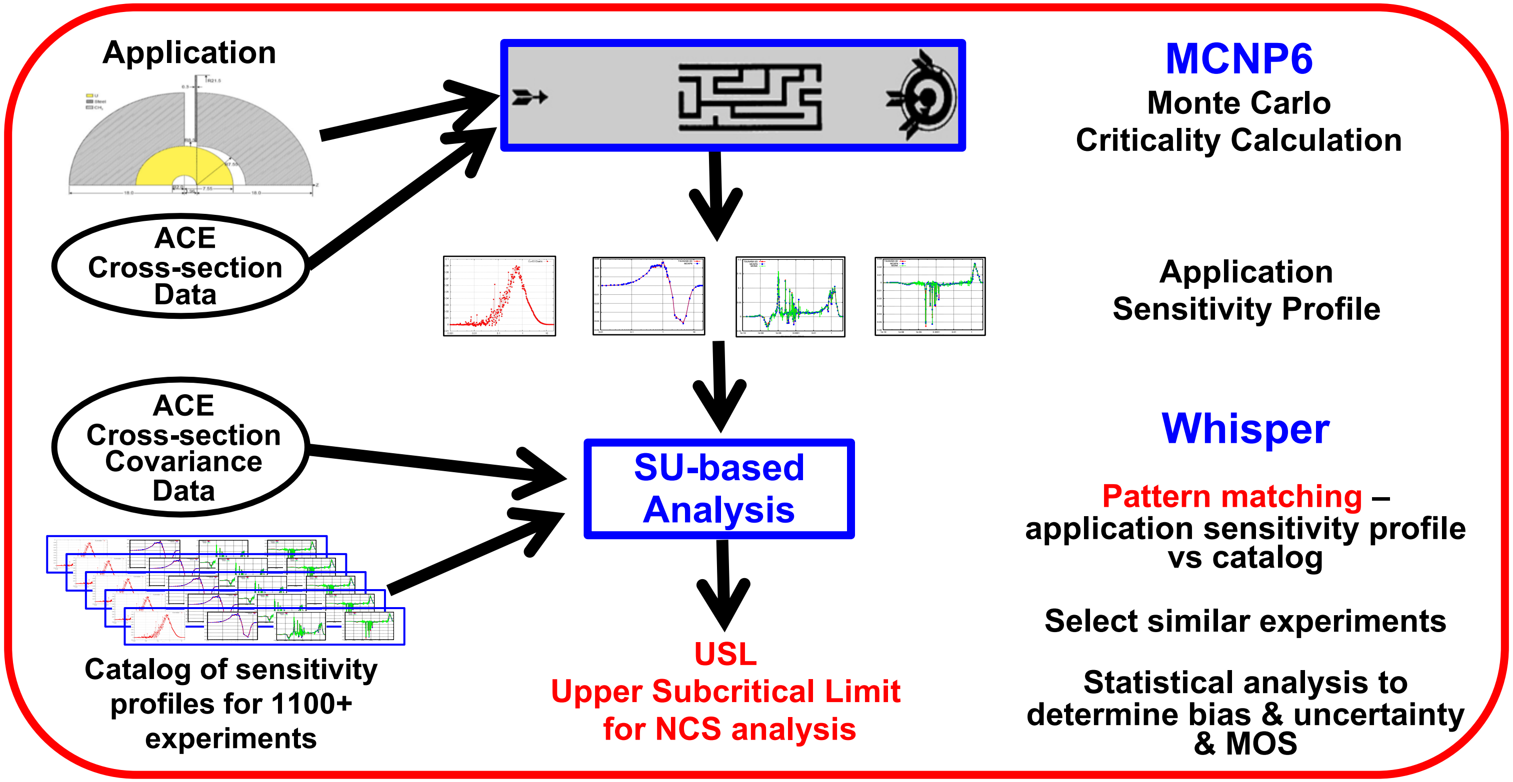
Supported on Mac, Linux, Windows
Used for ~1,000,000 processor-hours / month at LANL

Frequent V&V testing for NCS applications

Bottom Line:
Switch to MCNP6.2
Download ENDF-B/VIII.0 ACE files at LANL Nuclear Data Team website

MCNP6 & Whisper Status (2)

- **Whisper-1.1 – Included in MCNP6.2 RSICC Release**
  - No real coding changes in 2018 (only for research purposes)
  - For V&V work, tested benchmarks with ENDF/B-VIII
  - To complete a full upgrade to ENDF/B-VIII.0, we will need to include updated covariance data (looking at FY19 for this task)



Verification
&
Validation

MCNP Verification & Validation (1)

Verification Suites

- REGRESSION
  - Run by developers for QA checking
- VERIFICATION_KEFF
  - Analytic benchmarks, exact solutions for k_{eff}
  - Continuous-energy & multigroup
- VERIFICATION_GENTIME
  - 10 benchmarks for reactor kinetics parameters
- KOBAYASHI
  - 6 void & duct streaming problems, with point detectors, exact solutions
- Ganapol Benchmarks
  - Exact, semi-analytic benchmark problems
  - Fixed source, not criticality
- Gonzales Benchmark
  - Exact analytic benchmark with elastic scatter, including free-gas scatter

Validation Suites

- VALIDATION_CRITICALITY
  - 31 ICSBEP Cases, too small for serious V&V
  - Today, used for
    - Code-to-code verification, with real NCS problems & data
    - Compiler-to-compiler verification, with real NCS problems & data
    - Timing tests for optimizing MCNP coding & threading
  - Run at least weekly, to check MCNP6 for NCS
- VALIDATION_CRIT_EXPANDED
  - 119 ICSBEP Cases
  - Broad-range validation, for developers
- VALIDATION_CRIT_WHISPER
  - 1101 ICSBEP Cases
  - Used with Whisper methodology for serious validation
  - Will be expanded, as time permits
    - Sandia benchmarks
    - Others

MCNP Verification & Validation (2)

- Criticality Validation Suites with ENDF/B-VIII.0
  - VALIDATION_CRIT_EXTENDED
  - WHISPER

- Results ENDF/B-VIII.0 improved for:
  - Pu overall PU-SOL
  - HEU overall HEU-MET
  - MIX
  - IEU
  - ^{233}U-MET-FAST
- Preliminary results for other series appear to be acceptable

Suite	# OF CASES	ENDF/B-VII.1			ENDF/B-VIII.0		
		RMS %	Average C/E	C/E STD	RMS %	Average C/E	C/E STD
VALIDATION_CRIT_EXTENDED	**119**	**0.42**	**0.9994**	**0.0039**	**0.41**	**0.9986**	**0.0038**
WHISPER	**1101**	**0.74**	**1.0017**	**0.0072**	**0.76**	**1.0003**	**0.0076**
WHISPER: Pu	**262**	**0.97**	**1.0062**	**0.0075**	**0.95**	**1.0035**	**0.0088**
WHISPER: PU-COMP	36	2.06	1.0177	0.0106	2.14	1.0186	0.0108
WHISPER: PU-MET	68	0.66	1.0040	0.0054	0.73	1.0039	0.0063
WHISPER: PU-SOL	158	0.64	1.0045	0.0045	0.47	0.9999	0.0047
WHISPER: HEU	**386**	**0.57**	**1.0016**	**0.0055**	**0.63**	**1.0009**	**0.0057**
WHISPER: HEU-COMP	26	1.50	1.0143	0.0046	1.57	1.0151	0.0044
WHISPER: HEU-MET	267	0.42	1.0009	0.0041	0.40	0.9999	0.0041
WHISPER: HEU-SOL	93	0.47	1.0000	0.0047	0.49	0.9998	0.0049
WHISPER: MIX	**73**	**0.70**	**1.0035**	**0.0060**	**0.61**	**1.0018**	**0.0058**
WHISPER: IEU	**13**	**0.43**	**1.0024**	**0.0038**	**0.32**	**1.0005**	**0.0033**
WHISPER: LEU	**209**	**0.28**	**0.9995**	**0.0028**	**0.28**	**0.9994**	**0.0027**
WHISPER: ^{233}U	**158**	**1.06**	**0.9964**	**0.0100**	**1.18**	**0.9939**	**0.0102**
WHISPER: ^{233}U: COMP-THERM	9	0.20	0.9995	0.0020	0.33	0.9971	0.0016
WHISPER: ^{233}U: MET-FAST	10	0.25	0.9982	0.0019	0.17	0.9993	0.0017
WHISPER: ^{233}U: SOL-INTER	33	1.72	0.9837	0.0056	1.99	0.9809	0.0056
WHISPER: ^{233}U: SOL-THERM	106	0.87	0.9999	0.0087	0.92	0.9971	0.0088

- See J. Alwin presentation

MCNP Verification & Validation (3)

- **Subcritical Multiplication Validation Suite**
- **Working with NEN-2 (J. Arthur, J. Hutchinson et al.) to assemble together inputs and post-processing scripts**
  - **An automated validation suite is the ultimate goal**
  - **Similar to the established V&V suites, can be used to determine if:**
    - Code, algorithm or bug fixes have an impact for these problems
    - Nuclear data changes (ENDF/B-VII.1 → ENDF/B-VIII.0) make a difference
    - Fission models like CGMF and/or FREYA can be used

- **In FY18 this project began:**
  - **Looking at BeRP-Ni, BeRP-W and SCRαP benchmarks**
  - **Paper submitted to the 2018 Advances in Nuclear Nonproliferation Technology and Policy Conference 2018, Wilmington NC**
    - J.A. Arthur, M.E. Rising, J.D. Hutchinson, A.T. McSpaden, R.M. Bahran, “Validation of MCNP6 Using Subcritical Benchmark Experiments” (LA-UR-18-24470).
  - **Presented at 2018 ANS Winter Meeting, Orlando FL, (LA-UR-18-30598)**

- **Currently working on automating the execution, post-processing and documentation of the subcritical multiplication benchmarks**

User Support, Training & Education

User Support & Training

- **User support**
  - **MCNP Forum - User-group, beginners & experts, ~ 1500 members**
  - **MCNP Website**
  - **MCNP Reference Collection, > 700 technical reports**
  - **Summer students (UNM, MIT, Michigan, RPI, Oregon St)**
  - **Direct support available for LANL NCS Division**
- **Conferences & Journals**
  - **Nuc Sci Eng, Annals of Nuc En, Prog Nuc En, JCTT, etc.**
  - **M&C-2015, ICNC-2015, PHYSOR-2016, ICTT25, NCSD-2017, RPSD-2018**
    - Many XCP-3 staff helped organize and host the meeting in Santa Fe, NM
  - **ANS …, Las Vegas, San Francisco, Washington, Philadelphia …**
  - **OECD/NEA Sub-groups (formerly known as Expert Groups)**
    - **New SG-6** on "Statistical tests for diagnosing fission source convergence and undersampling in Monte Carlo criticality calculations"
    - Led by Forrest Brown at LANL
- **Introductory (and Intermediate, new in FY19) MCNP Classes**
  - **Generally held onsite at LANL ~6 times/year**
  - **Also new in FY19, teaching classes at OECD/NEA ~4 weeks/year**

Training & Education

- Sensitivity-Uncertainty Methods for NCS Validation
  - 1-day class, at DOE sites, joint effort with ORNL (SRS in FY18)
  - Theory, Practice, MCNP6-Whisper & SCALE-Tsunami-Tsurfer
- Criticality Calculations with MCNP6
  - 4-day class with hands-on examples
  - LANL 2x/year, other DOE sites on request (Y-12 in FY18)
- Monte Carlo course at University of New Mexico
  - 1-semester class for senior undergrads & new grad students
  - Includes some students in LANL NCSD intern program
  - Theory & practical MCNP usage, emphasis on criticality problems
  - Lecture notes are on the MCNP website, in Reference Collection
- Advanced Monte Carlo course at University of New Mexico
  - 1-semester class for graduate students
  - Also presented at LANL to Monte Carlo developers
  - Advanced & important topics, not found anywhere else
  - Lecture notes are on the MCNP website, in Reference Collection

R&D Work in Progress

Automated Acceleration & Convergence Testing
Impact of Outliers on NCS Validation and USLs
Machine Learning Methods using Nuclear Data Sensitivities
Correlated Fission Multiplicity in Critical & Subcritical Simulations
Region-wise Sensitivities for NCS Validation

Student Mentoring to Support R&D Work

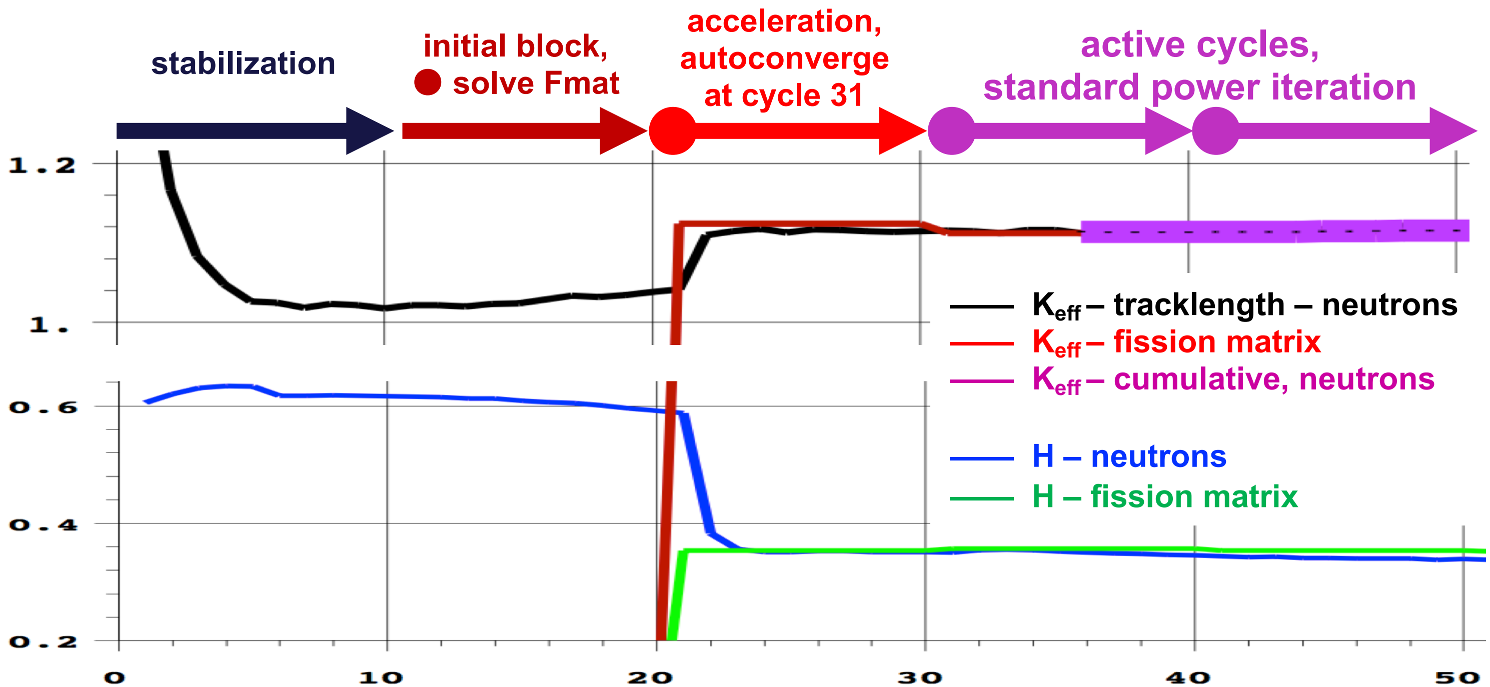
- **LANL Postdocs (both converted to staff now)**
  - Colin Josey – alpha methods, fission matrix, etc
  - Tim Burke – kernel density estimator tallies, heterogeneous computing

- **Summer interns & Graduate Research Associates**
  - UNM: Dan Timmons – fission neutron multiplicity
  - UNM: Bobbi Riedel – region-wise sensitivities
  - Oregon St: Pavel Grechanuk – analytic benchmarks, machine learning

- **Other**
  - SNL/UNM: Shawn Henderson – sparse fission matrix

R&D – Automated Acceleration & Convergence Testing

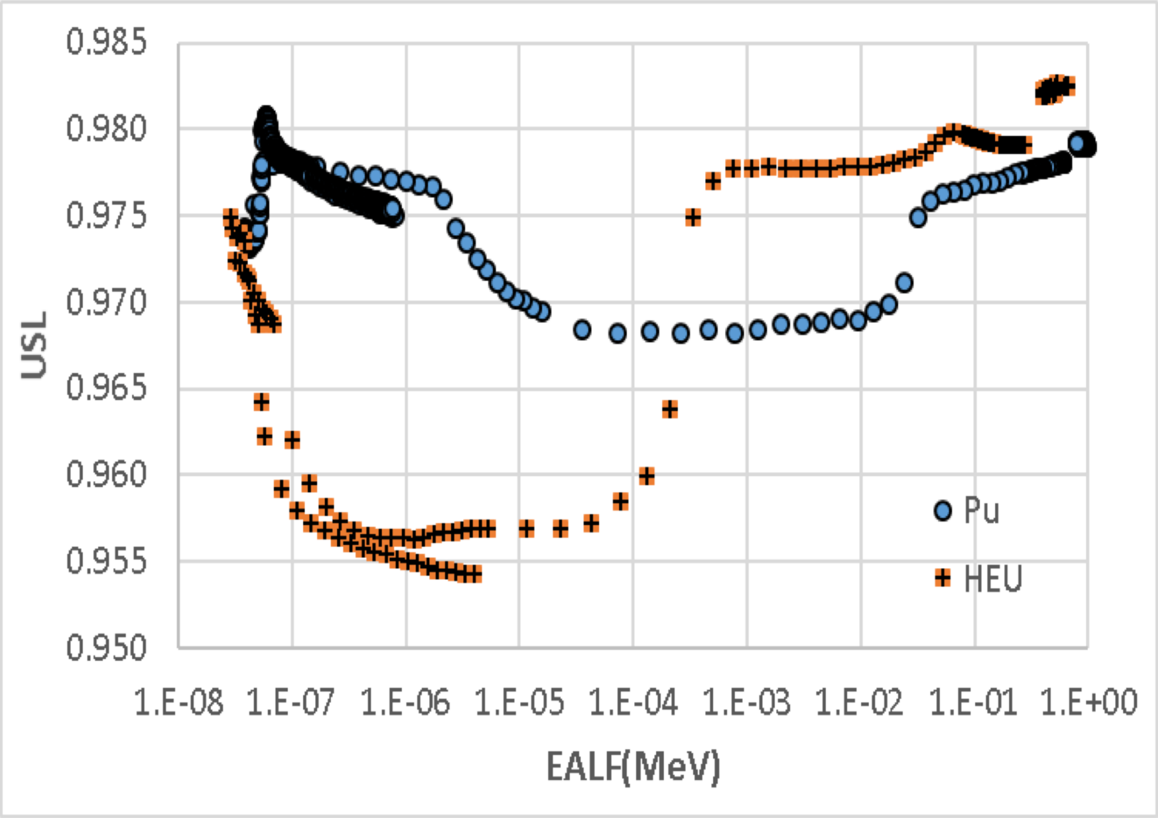
- Completely automate NCS criticality calculations
  - Accelerate convergence of fission source & k-effective
  - Statistical testing for convergence
  - Automatically switch to active cycles
  - Tests on adequate number of neutrons/cycle
- See F. Brown presentation



R&D – Impact of Outliers on NCS Validation and USLs

- See J. Alwin presentation

Whisper Baseline USL for Pu and HEU Systems

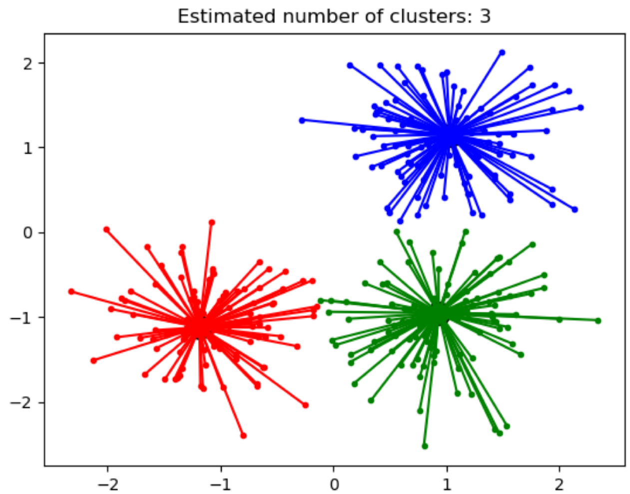


USL Difference: |USL $_{exclusions}$ – USL $_{all\ benchmarks}$|	
Pu metals	0.00021
Pu oxides	0.00234
Pu solutions	0.00026
HEU metals	0.00050
HEU oxides	0.00208
HEU solutions	0.00307

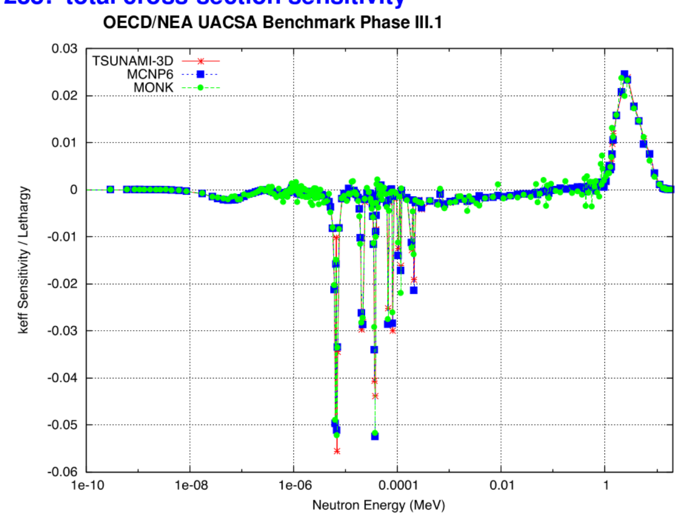
- **Impact of excluding benchmark outliers on NCS Validation**
- **Minimal difference in baseline USL whether outliers are included or excluded**
- **Neither method is consistently conservative, depends on system**

R&D – Machine Learning & Nuclear Data Sensitivities

- **Nuclear data sensitivity profiles describe how a critical system depends on the nuclear data**
- **Question: Is it possible to use Machine Learning algorithms and nuclear data sensitivity profiles to detect hidden patterns in the nuclear data? (See P. Talou & M. Rising presentation)**
- **Clustering can be used to find inherent relationships in the data**
  - Objects in the same cluster are similar to each other
  - Used to find groups of benchmarks that have similar sensitivity profiles



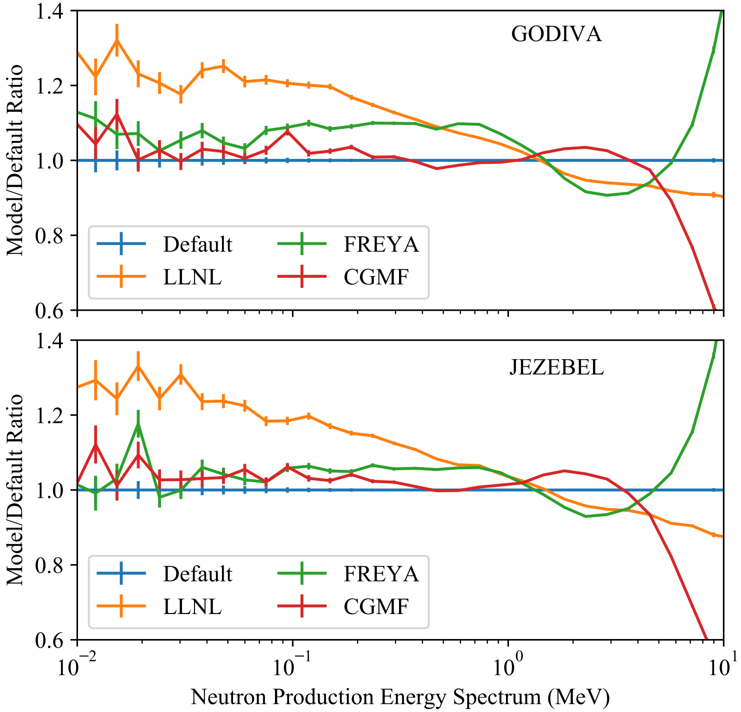
U-238: total cross-section sensitivity

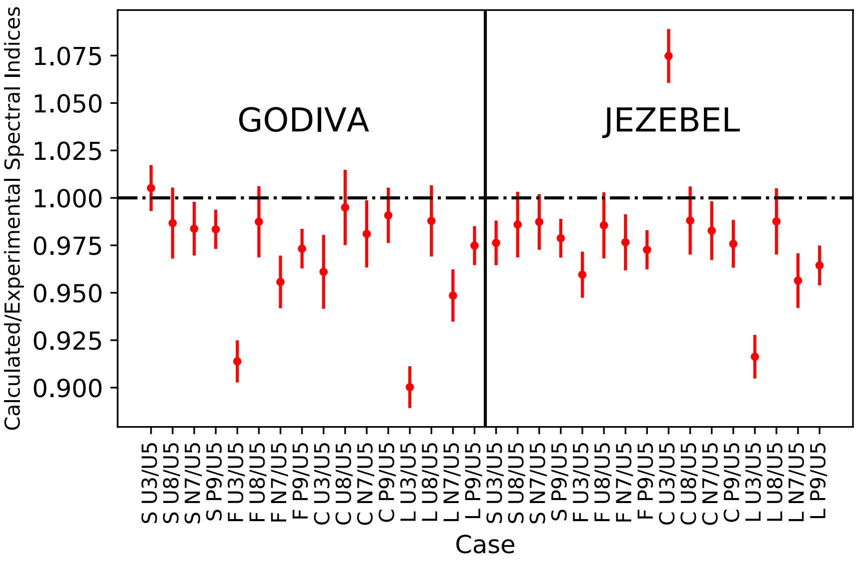


R&D – Correlated Fission Multiplicity in Criticality

- For nuclear nonproliferation and safeguards needs, the correlated fission multiplicity models, CGMF and FREYA, are in MCNP6.2
  - For fixed-source problems only (disabled for KCODE calculations)

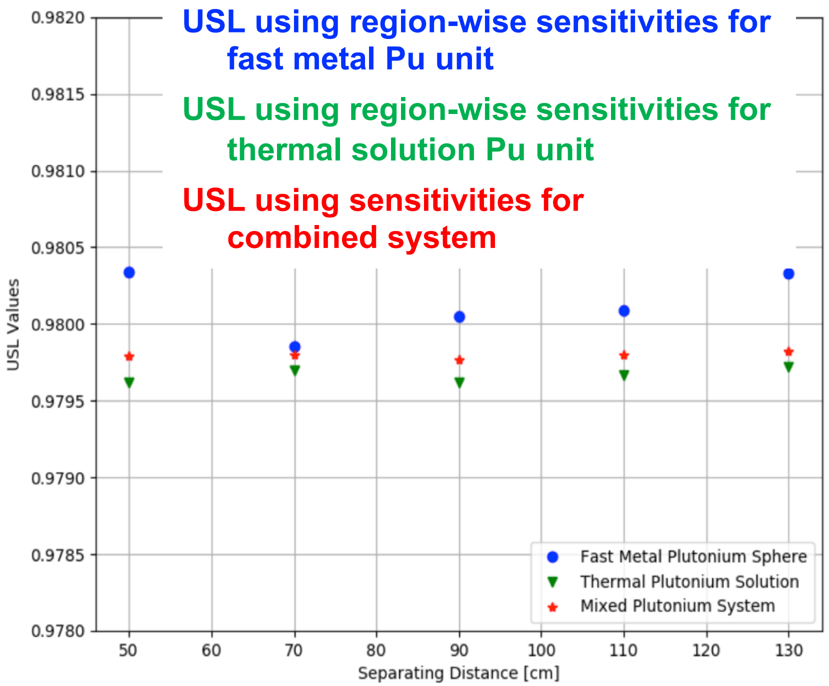
- Question: How do these models impact criticality calculations?
  - Multiplicity distribution of neutrons and gamma rays
  - Multiplicity-dependent energy spectra
  - Angular emission from fission fragments





R&D – Region-wise Sensitivities for NCS Validation

- **Standard sensitivity-uncertainty methods**
  - Based on sensitivity profiles averaged over entire problem
  - MCNP6-Whisper, SCALE-tsunami-tsurfer
- **What if there are multiple fissile units in a problem?**
  - Averaged SU-analysis methods may be inappropriate
  - What to do about HEU, Pu, U233 units in same storage vault?
- **Proposal: Use region-wise sensitivity profiles**
  - MCNP6 can already do this
  - Need to investigate practical applications
- **R&D activities**
  - Examine sensitivity profile for a unit as function of separation from other units
  - Investigate mods to Whisper to permit coupling coefficients or sensitivity profile modifiers based on separation distances



MCNP Code Modernization

MCNP Code Modernization (1)

- **Since the time of the MCNP5 and MCNPX merger, the complexity of the code and all of its internal dependencies has remained at a generally high level with a steep learning curve**
  - **For example, it used to be possible for summer student internship projects to be focused on developing a new capability directly in the MCNP5 source code … this is <u>nearly impossible</u> in MCNP6 today**
  - **This also means that we have seen a large increase in code development team time and effort required to do seemingly easy tasks like:**
    - minor improvements
    - routine maintenance
    - testing
    - code releases

- **For the long-term future and sustainability of MCNP**
  - **We are currently focused on modernization of the code including our development practices**

MCNP Code Modernization (2)

- **General MCNP Modernization Goals:**

1) Improve code development practices

- Adopt more industry-standard tools to get the job done
  - New staff are already accustomed to many of these tools
  - Better practices will certainly maintain or improve our SQA requirements
- Succeeding here will make the following goals more easily attainable

2) Improve and reorganize code infrastructure and data flow

- Top-down approach to managing how the code executes and how data is managed throughout a calculation
- Isolating and understanding these top-level operations will facilitate a more narrowed view into the next level of components, so that unnecessary dependencies can be pulled apart more easily

3) Improve code data structures

- Bottom-up approach to organizing and structuring common, fundamental data together into immediately recognizable units
- Much of this kind of work can be done generically in a library, such that it is reusable for other code projects as well (facilitates leveraging of funding and resources for common needs between programs)

MCNP Code Modernization (3)

- **In FY18**
  - **MCNP6 is now fully Fortran 2008 and C++17 standards compliant**
  - **Adopted modern software development tools**
    - ✓ Version control system – CVS ➔ git
    - ✓ Build, test and package software – GNU Make ➔ CMake & CTest
    - ✓ Repository management / code reviews – TeamForge / Gerrit ➔ Bitbucket
    - ✓ Artifact / issue tracking – TeamForge ➔ Jira
    - ✓ Team communication / wiki – TeamForge ➔ Confluence
    - ✓ Continuous build and testing system – CBTS ➔ Jenkins Test Servers
  - **Getting away from “home-grown” build and test systems was not a trivial task (1600+ tests converted from gmake to ctest), but it was essential so developers can spend more of their time on the important tasks ahead**
  - **Wrote a generic, standalone, unit tested C++ sources and distributions library that, when finally integrated into MCNP, will replace the general source (SDEF) sampling and distribution routines**

MCNP Code Modernization (4)

- **Examples of present work and next steps in modernization**
  - **Improved tools and development practices are already in use**
  - **Infrastructure improvements**
    - Looking into runtpe and various output file upgrades (HDF5?)
    - Reorganizing source and global into common components
  - **Data structure improvements**
    - Rewriting PTRAC capability right now with improved buffering and parallelism

- **There are many other tasks currently or soon to be underway!**

Summary

- **MCNP & Whisper releases**
  - MCNP5 is no longer supported,   cannot use continuous S(α,β)
  - MCNP6.2 & Whisper-1.1 release – March 2018
- **Whisper – Sensitivity-uncertainty methods**
  - Whisper methods for validation & USLs are important to LANL & other DOE sites
  - Training is available
  - Outstanding success due to long-range vision & support from NCSP
- **Ongoing – user support, training, and education**
- **R&D work in progress – several areas**
  - Automated Acceleration & Convergence Testing
  - Impact of Outliers on NCS Validation and USLs
  - Machine Learning Methods using Nuclear Data Sensitivities
  - Correlated Fission Multiplicity in Critical & Subcritical Simulations
  - Region-wise Sensitivities for NCS Validation
- **MCNP Code Modernization**
  - Code development practices and tools have recently been upgraded
  - Using both a top-down and bottom-up approach to addressing different issues within the code

Acknowledgements

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Questions ?