# MCNP® Progress for NCSP

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

NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

Los Alamos
NATIONAL LABORATORY
EST. 1943

# Abstract


## MCNP® Progress for NCSP

**Michael Rising, Forrest Brown, Jennifer Alwin**

**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 2017 and early FY 2018. 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 2020 & code modernization**


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

# MCNP® Progress for NCSP

## US DOE-NNSA Nuclear Criticality Safety Program –

### What have we done for you lately (FY 2017, FY 2018) ?

- **Overview of LANL Analytical Methods Work for NCSP**
- **MCNP6 & Whisper Status**
- **Verification / Validation**
- **User Support, Training & Education**
- **R&D Work in Progress**
  - Region-wise Sensitivities
  - Sparse-storage Fission Matrix
  - New Alpha-Eigenvalue Methods
  - Machine Learning to Predict Bias
  - Presence of Chlorine in Process Operations
- **MCNP 2020 & Code Modernization**

# Overview of LANL Analytical Methods Work for NCSP

In-depth experience & expertise in all areas:
theory, codes, computers, applications,
user support, teaching, design, validation, …..

## Forrest Brown

Whisper support
MCNP – physics, algorithms
MCNP – MCNP 2020, parallel
Teaching – Professor at UNM
Collab – SNL, UNM, RPI, Mich, MIT

## Michael Rising

Fission neutron multiplicity
MCNP – physics, code
MCNP – MCNP 2020
Summer intern – Oregon St
Collaboration – SNL, UNM

## Jennifer Alwin

Criticality & NCS validation
MCNP – Whisper vs ANS-8.24
MCNP – solution chemistry
PF4-NCS support & training
Collaboration – SNL

## All – Ongoing Work

MCNP – release & NCS testing
MCNP – maintenance & bug-fixes
MCNP – benchmark catalogs
Training – MCNP criticality classes
Training – NCS validation, SU methods
Verification-validation
Criticality documentation
Best Practices for Criticality Calcs
MCNP Reference Collection
MCNP Forum email users group
MCNP web site
User support

Some activities are partially funded by other programs

# 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

- ***Some* of the MCNP6.2 new features**
  - Longer input lines, up to 128 characters
  - Warning message regarding bias if using < 10,000 neutrons/cycle
  - MCNPTools, ISC, & other improved utilities
  - Data and code bug fixes (described later)

# MCNP6 & Whisper Status (2)

## MCNP6.2 Release

- **2016**
  - Code work & V&V finished in Spring
  - Delays in finishing User-Manual, Test documents, Release Notes
  - Long delay in getting approval to issue User Manual as publicly available LA-UR report, instead of controlled publication
- **2017**
  - Documentation work & approval finished in Summer
  - Routine request to lab lawyers to approve copyright statement
  - Lawyers being lawyers, they discovered

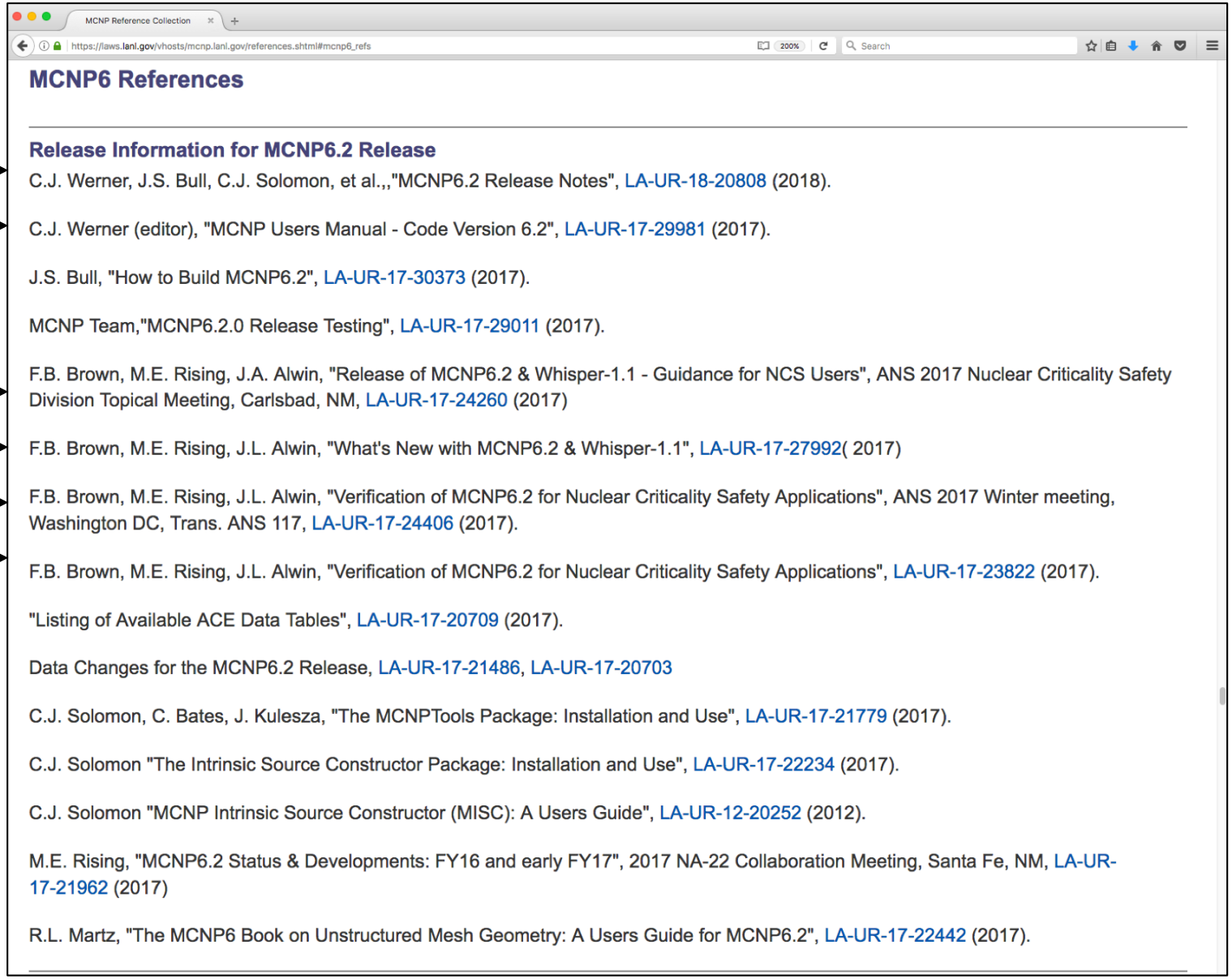
    The LANL Prime Contract requires all funding sponsors for a computer code to explicitly approve any release
  - Immediate approval from DOE-NNSA ASC & NCSP
  - Long delays from DHS
- **2018**
  - Approval from DHS, pending extra Readme file with legalease...
  - LANL lawyers at work again
  - Finally, release to RSICC on 2018-03-12

# MCNP6 & Whisper Status (3)

- **MCNP6.2 Release Information on website: mcnp.lanl.gov**

**Manual is now unlimited release (not export controlled)**

**All NCSP-related release documents completed last year, in FY17**



MCNP Reference Collection

https://laws.lanl.gov/vhosts/mcnp.lanl.gov/references.shtml#mcnp6_refs

## MCNP6 References

### Release Information for MCNP6.2 Release

C.J. Werner, J.S. Bull, C.J. Solomon, et al.,,"MCNP6.2 Release Notes", LA-UR-18-20808 (2018).

C.J. Werner (editor), "MCNP Users Manual - Code Version 6.2", LA-UR-17-29981 (2017).

J.S. Bull, "How to Build MCNP6.2", LA-UR-17-30373 (2017).

MCNP Team,"MCNP6.2.0 Release Testing", LA-UR-17-29011 (2017).

F.B. Brown, M.E. Rising, J.A. Alwin, "Release of MCNP6.2 & Whisper-1.1 - Guidance for NCS Users", ANS 2017 Nuclear Criticality Safety Division Topical Meeting, Carlsbad, NM, LA-UR-17-24260 (2017)

F.B. Brown, M.E. Rising, J.L. Alwin, "What's New with MCNP6.2 & Whisper-1.1", LA-UR-17-27992( 2017)

F.B. Brown, M.E. Rising, J.L. Alwin, "Verification of MCNP6.2 for Nuclear Criticality Safety Applications", ANS 2017 Winter meeting, Washington DC, Trans. ANS 117, LA-UR-17-24406 (2017).

F.B. Brown, M.E. Rising, J.L. Alwin, "Verification of MCNP6.2 for Nuclear Criticality Safety Applications", LA-UR-17-23822 (2017).

"Listing of Available ACE Data Tables", LA-UR-17-20709 (2017).

Data Changes for the MCNP6.2 Release, LA-UR-17-21486, LA-UR-17-20703

C.J. Solomon, C. Bates, J. Kulesza, "The MCNPTools Package: Installation and Use", LA-UR-17-21779 (2017).

C.J. Solomon "The Intrinsic Source Constructor Package: Installation and Use", LA-UR-17-22234 (2017).

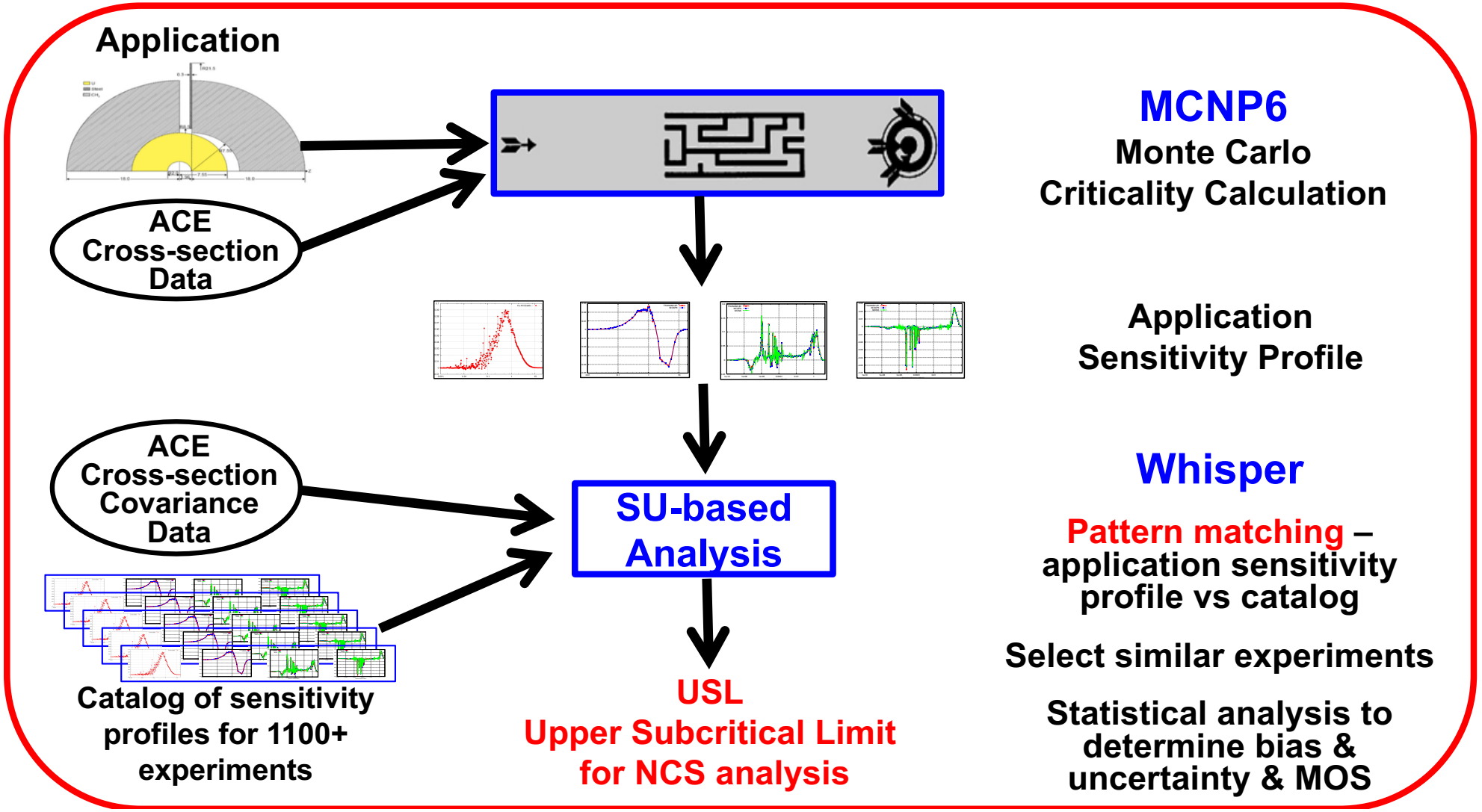
C.J. Solomon "MCNP Intrinsic Source Constructor (MISC): A Users Guide", LA-UR-12-20252 (2012).

M.E. Rising, "MCNP6.2 Status & Developments: FY16 and early FY17", 2017 NA-22 Collaboration Meeting, Santa Fe, NM, LA-UR-17-21962 (2017)

R.L. Martz, "The MCNP6 Book on Unstructured Mesh Geometry: A Users Guide for MCNP6.2", LA-UR-17-22442 (2017).

# MCNP6 & Whisper Status (4)

- **Whisper-1.1 – 1st Public Release**
  - Coding, 1101 ICSBEP benchmarks, scripts, & 50+ documents
  - Portable to Mac, Linux, Windows



# 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)

- **What changes in MCNP6.2 do NCS users need to be aware of?**
  - **Changes in MCNP6.2 Coding**
    - Compliance with Fortran 2003 standard
    - Continuous S(α,β) numerics (fixed since MCNP6.1.1 release)
    - Coincident surface treatment – containers with rotated universe
      - New method causes some small differences
    - k-adjoint first k-effective estimate
      - Fix causes minor adjoint-weighted reactor kinetics parameter differences
  - **Changes in Nuclear Data Libraries (ENDF/B-VII.1)**
    - Revised Hydrogen $(n,\gamma)$ production data
      - Use 1001.[90-96]c in place of 1001.[80-86]c
    - $SiO_2$ S(α,β) thermal scattering data
      - Use sio2.[10-16]t in place of sio2.[30-36]t
    - Zirc-Hydride S(α,β) thermal scattering data at 1200K
      - Use h-zr.28t in place of h-zr.27t
    - New xsdir_mcnp6.2 makes the above fixed data the default
- **All of these minor issues have been extensively verified & tested**

# 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, others**
  - **M&C-2015, ICNC-2015, PHYSOR-2016, ICTT25, NCSD-2017**
    - Presented all-day workshop on MCNP-Whisper and three full papers
  - **ANS …, San Antonio, Washington, Las Vegas, San Francisco, …**
  - **OECD Expert Groups - Advanced Monte Carlo, Sensitivity-Uncertainty**

- **Introductory MCNP Classes**
  - **Generally held onsite at LANL ~6 times/year**
  - **Several upcoming seats occupied by LANL NCS student interns**
  - **Beginning to offer *some* offsite classes**
    - Presented 1 NCSU class in Dec. 2017

# Training & Education

- **Sensitivity-Uncertainty Methods for NCS Validation**
  - 1-day class, at DOE sites, joint effort with ORNL (Y-12 in FY17)
  - 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 (PNNL in FY17)
- **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

Region-wise Sensitivities

Sparse-storage Fission Matrix

New Alpha-Eigenvalue Methods

Machine Learning to Predict Bias

Presence of Chlorine in Process Operations

New Random Number Package

Correlated Fission Multiplicity

(If Time Permits)

# Student Mentoring to Support R&D Work

- **LANL Postdocs**
  - Colin Josey – alpha methods, RNGs, 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 Grechanek – analytic benchmarks, machine learning
- **Other**
  - SNL/UNM: Shawn Henderson – sparse fission matrix

# R&D – Region-wise Sensitivities

- **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

# R&D – Sparse-storage Fission Matrix

- **Fission matrix method for k-effective problems**
  - Theoretically sound, analyzed since 1950s
  - Impractical for general use due to memory-size limitations

- **Sparse-storage fission matrix**
  - Breakthrough advance in 2010s by Brown, Carney, Kiedrowski
  - Removes memory limits, can apply detailed treatment to any problem
  - Can provide reference solution even during inactive k-cycles
  - Immune to correlation, clustering, & bias problems caused by repeated renormalization of neutron distribution each cycle

- **Proposal: Use sparse-storage fission matrix for all problems**
  - **Automated convergence test** – neutron distribution vs fission matrix reference solution
  - **Population size test** - determine if (neutrons/cycle) is large enough to prevent undersampling & clustering problems
  - **Accelerate convergence** - Use fission matrix reference solution to accelerate convergence of neutron distribution

# R&D – New Alpha-Eigenvalue Methods

- **MCNP6 calculation of alpha-eigenvalues**
  - Alpha-mode calculations of time behavior after fast burst or scram
  - Longstanding feature of in-house LANL versions of MCNP
  - Not part of MCNP distribution through RSICC
  - Available to other DOE-sites on request from XCP-3

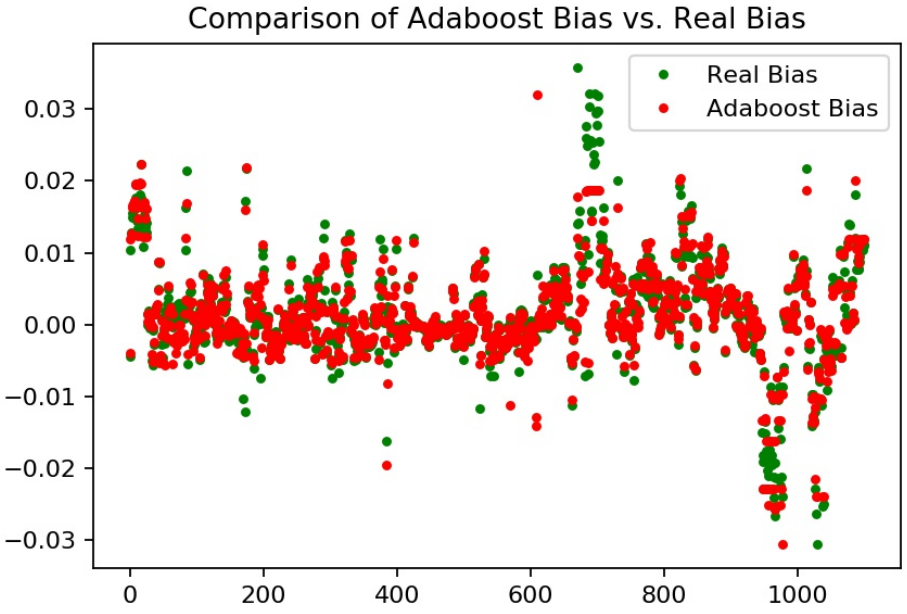
- **Basic algorithm improvements**
  - Conventional k-alpha search is not robust, requires careful selection of algorithm parameters, & only works for prompt neutrons
  - Improvements
    - Accurate integral-based method for estimating alpha
    - Improved method for alpha-updates during iterations
    - Incorporate delayed neutrons (previously, only prompt neutrons)

- **Status**
  - Demonstrated effectiveness in research mods to MCNP6
  - Plan to integrate into production MCNP6 in 2018
  - Extensive LANL testing, public release

# R&D – Machine Learning to Predict Bias

- **Whisper can be used to help determine a baseline USL for a given application (including bias + uncertainty & additional margin)**
  - **Uses benchmark catalogue of 1100+ calculations with sensitivities**
  - **Conservative estimate of bias + uncertainty**
  - **GLLS used to quantify additional margin of subcriticality**

- **Question: Is it possible to use machine learning and the Whisper sensitivity data to accurately predict the bias in $k_{eff}$?**
  - **Possibly useful for new designs**
  - **Obtain importance of sensitivity data to the bias in $k_{eff}$**
  - **Provide feedback to nuclear data community on what can be improved**




| Thermal (0 - 0.625 ev) | Intermediate (1.0 ev - 0.1 Mev) | Fast (0.4 Mev - 20 Mev) |
|---|---|---|
| Carbon, n-gamma, 0.014562 | U-233, n-gamma, 0.018457 | U-233, fission, 0.015264 |
| U-233, total nu, 0.011437 | U-233, fission, 0.015724 | U-233, inelastic, 0.013543 |
| U-233, n-gamma, 0.010641 | U-233, total nu, 0.012844 | U-233, n-gamma, 0.012739 |
| U-234 n-gamma, 0.009479 | U-234, n-gamma, 0.011945 | U-233, total nu, 0.012644 |
| H-1 n-gamma, 0.009069 | Pu-239, n-gamma, 0.011687 | F-19, inelastic, 0.010355 |

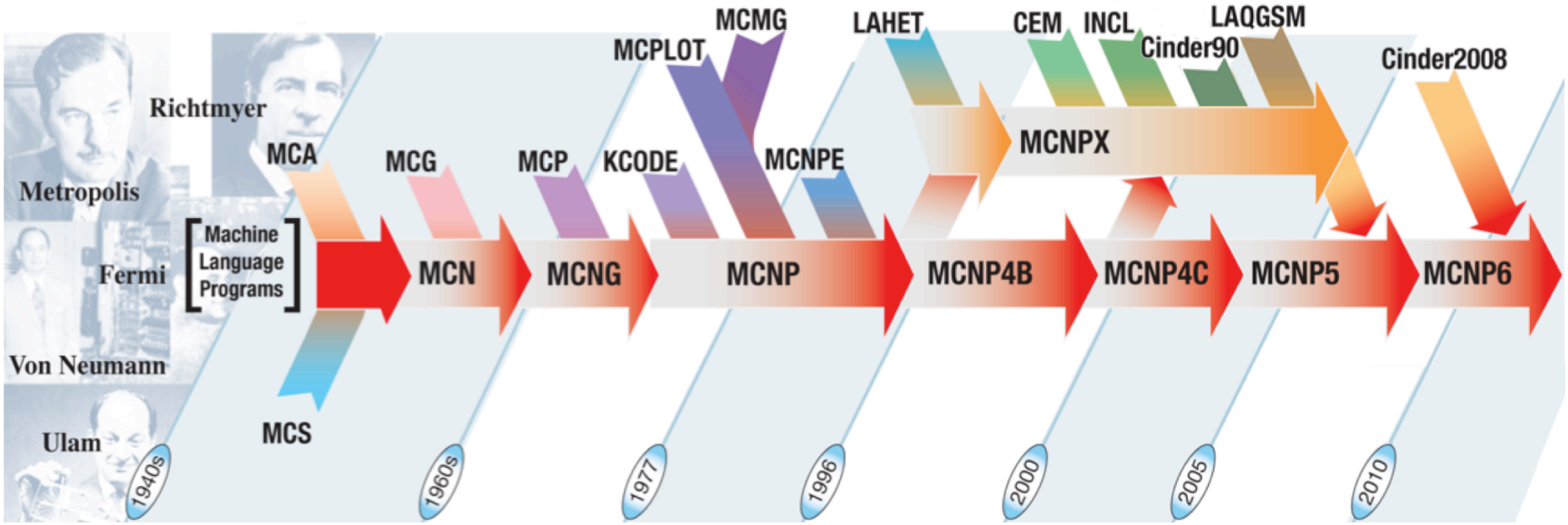
# R&D – Presence of Chlorine in Process Operations

- **In situ neutron multiplication measurements**
  - **Calculate subcritical multiplication & compare in situ measurements**
  - **Predict k-effective for abnormal conditions and quantify existing margin and conservatisms, evaluation model vs. practical conditions**
    - Pu metal-water mix vs. Pu chloride solutions
    - PVDF (polyvinyl difluoride) tanks
    - Presence of gadolinium oxide in tank walls
- **Development of solution density laws**
  - **Similar methodology to nitrate Isopiestic law developed by IRSN/CEA**
  - **Work underway to experimentally measure binary data for plutonium chloride solutions**
- **Proposed critical experiments for validation of chlorine**
  - **Whisper used to help design critical experiment**
  - **Determine if proposed experiment is within "area of applicability" for process operations**
- **Whisper used to help determine similarity to existing benchmark experiments, leading to recommended baseline USL**
  - **Can also help quantify additional area of applicability margin to account for limited data**

# MCNP 2020 & Code Modernization

# MCNP 2020 & Code Modernization (1)

- **The state of MCNP6.2**
  - The long (and occasionally windy) road to today




- **Currently, the code base includes:**
  - 431K lines of code + 88K lines of comments ~ 500K total
  - ~2-3 FTE from NCSP + ~6-7 FTE from ASC / Institutional ~ 9 FTE total

- **This is a big job for all of us – need more people**
  - We want the best and brightest, of course
  - Young staff are used to and expect more modern code practices!

# MCNP 2020 & Code Modernization (2)

- At LANL, there exists a strong will to see MCNP succeed
- How do we (curators of the code) setup for long term success?
  - Create a code modernization plan (under development)
  - Improve code development practices as a team
    - Code design documentation and prototyping practices
    - Peer-review and testing of all integrated code
    - Complete documentation of all code work
    - With all of these improved team processes documented and in place leads to improved SQA
  - Adopt modern software development tools
    - ✓ Version control system – CVS ➔ git
    - ✓ Build, test and package software – GNU Make ➔ CMake
    - Repository management / code reviews – TeamForge / Gerrit ➔ ???
    - Artifact / ticket tracking – TeamForge ➔ ???
    - Continuous build and testing system – CBTS ➔ ???

# MCNP 2020 & Code Modernization (3)

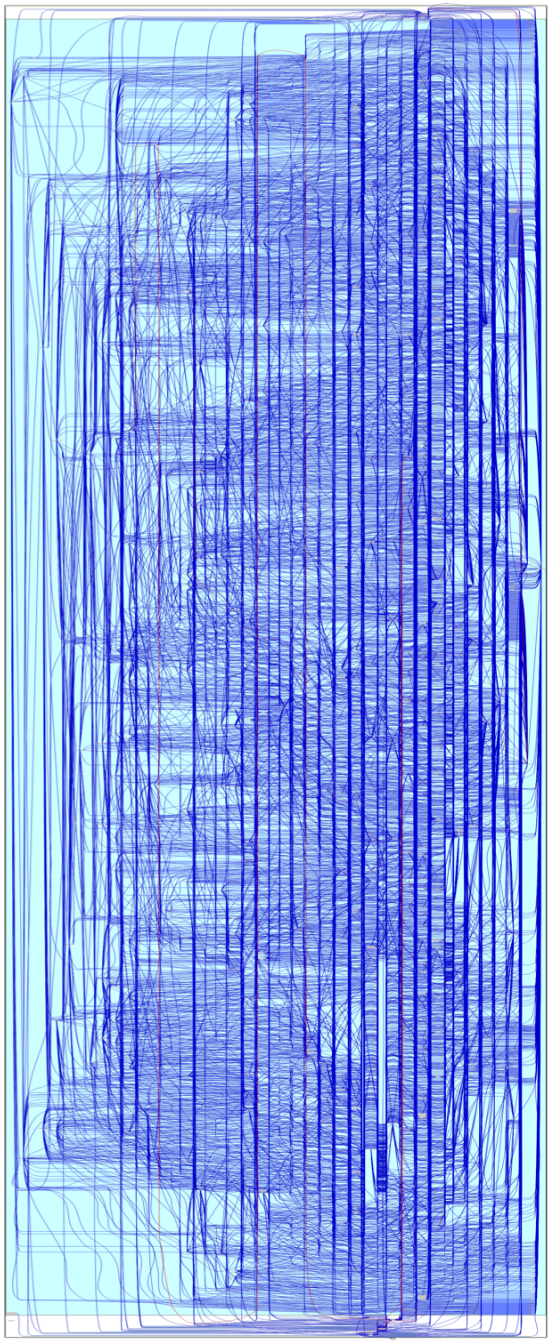
- **With all of the history of MCNP comes…**

**… many benefits**

- **Very feature-rich, many applications possible**
- **Extensive testing (90% coverage of code)**
- **Validation for important applications like NCS**
- **Expert experience and guidance available**

**… many challenges**

- **A tangled mess of source code, dependencies, etc. (see dependency graph ➔)**
  - No modularity – need to break dependencies
  - Unintended side-effects when calling a function
- **Diminished knowledge of some features**
- **Structural upgrades sorely needed**
  - Remove cryptic variable naming (2-3 letter variables)
  - Organize data structures in a logical way



# MCNP 2020 & Code Modernization (4)

- **MCNP 2020 & Code Modernization**
  - **Improve performance (MCNP 2020)**
    - ✓ Algorithmic improvements to speedup criticality calculations
  - **Upgrade core MCNP6 software (both, kind of)**
    - **Evolution, not revolution**
    - **Restructure, clean up code & data structures, standards compliance**
    - **Reduce future costs for development & maintenance**
  - **Prepare for future (both)**
    - MCNP 2020: new computers – massive parallel, but less memory per core
    - MCNP 2020: improve MPI & thread parallelism
    - Code Modernization: prepare code base to be more manageable and sustainable for future developers & platforms
- **The MCNP 2020 & general code modernization plans are closely associated with each other with many common goals**
- **NCSP support for the future of MCNP is invaluable**

# Summary (1)

- **MCNP releases**
  - **MCNP5 is no longer supported, cannot use continuous S(α,β)**
  - **MCNP6.1, MCNP6.1.1, & ENDF/B-VII.1 released in 2013 & 2014**
  - **MCNP6.2 & Whisper-1.1 release – March 2018**
    - All basic KCODE criticality features same as for MCNP5 & MCNP6.1
    - MCNP6 speed improved by 1.2 – 4 X for crit-safety.
    - Thorough testing with NCS criticality suites

- **Whisper – Sensitivity-uncertainty methods**
  - **Whisper methods for validation & USLs are important to LANL & other DOE sites**
  - **Being used routinely in many areas**
  - **Training is available**
  - **Outstanding success due to long-range vision & support from NCSP**

- **Ongoing – user support, training, and education**

# Summary (2)

- **R&D work in progress – several areas**
  - **Region-wise Sensitivities**
  - **Sparse-storage Fission Matrix**
  - **New Alpha-Eigenvalue Methods**
  - **Machine Learning to Predict Bias**
  - **Presence of Chlorine in Process Operations**
  - **And Others: Random Number Generators, Fission Multiplicity, etc.**

- **MCNP 2020 & Code Modernization**
  - **Algorithmic developments are always needed**
    - Improve and/or maintain performance
    - New hardware requires better parallel schemes
  - **Attention to the source code base is badly needed**
    - General code cleanup
    - Reorganization to break dependencies
  - **Adoption of more modern practices will help**
    - Overall software quality
    - Attract the next generation of MCNP code developers

# Questions ?

# R&D – New Random Number Package

- **Current MCNP random number generator has been in use for 15 yr**
  - **Default: 48-bit RNG, period ~ $10^{14}$**
  - **6 options: 63-bit RNG, period ~ $10^{18}$**

  - **For a criticality calculation with 10 billion neutrons**
    - Default RNG: cycle through entire RNG period 22 times
    - Other RNGs: use only ~ 0.1% of RNG sequence

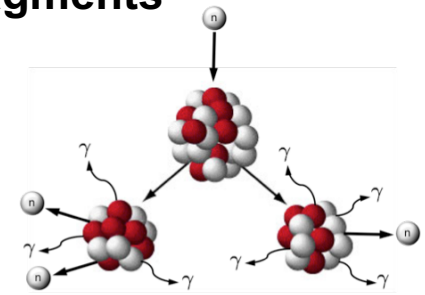
- **Proposal: Make the 63-bit RNG#2 the new default**
  - **Only a few lines of coding change**
  - **All results will change, but should agree within statistics**
  - **Need extensive V&V using standard MCNP criticality validation suites**
  - **Initial testing verifies that results agree within statistics**

- **Proposal: Modernized object-oriented RNG package**
  - **Alters algorithm to particle-owned RNG, instead of code-owned RNG**
  - **Easy to test & verify**

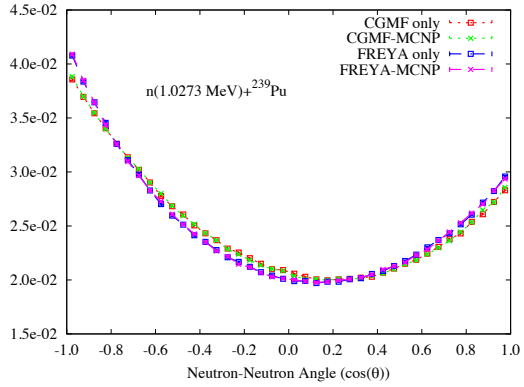
# R&D – Correlated Fission Multiplicity

## Secondary Emission from Fission

- Fixed-source nuclear nonproliferation and safeguards needs (NA-22)
- Neutron and Gamma-ray emission from fission fragments

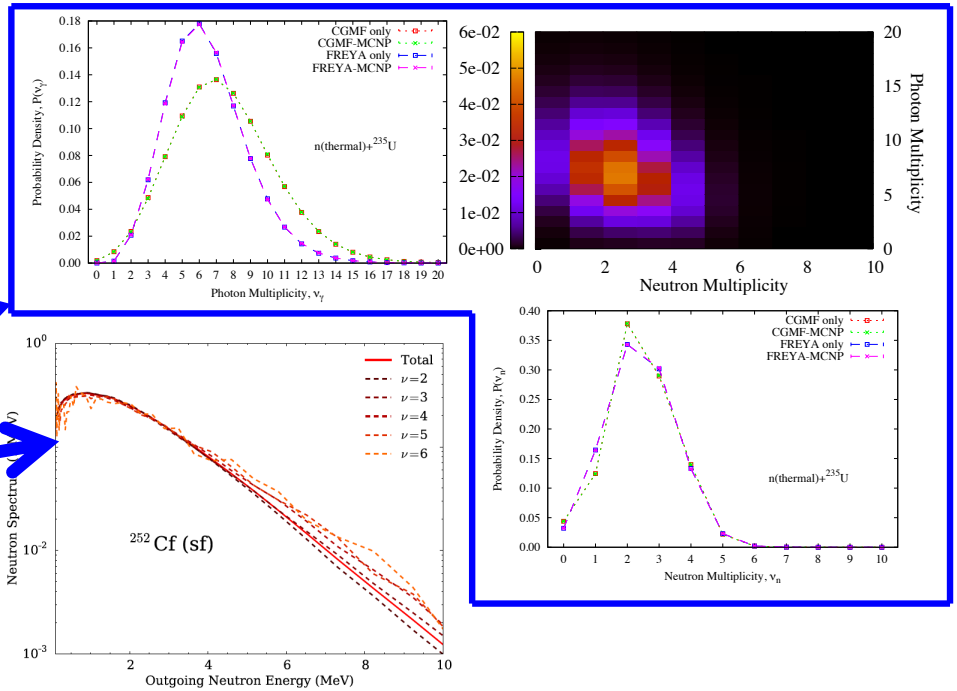


- Multiplicity distribution of neutrons and gamma rays
- Multiplicity-dependent energy spectra
- Angular emission from fission fragments




## What's New in MCNP6.2

- CGMF based on Monte Carlo Hauser-Feshbach theory (LANL)
- FREYA based on Monte Carlo Weisskopf theory (LBNL/LLNL)




- Looking at use in criticality calculations
- Planning to further investigate use in subcritical multiplication calculations