Title: MCNP Progress for NCSP

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MCNP Progress for NCSP

LA-UR-17-21840

Forrest Brown, Michael Rising, Jennifer Alwin

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

Forrest Brown, Michael Rising, 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 2016 and early FY 2017. Activities and accomplishments are summarized in five major areas:

- MCNP6 & Whisper status
- Verification and validation testing
- User support & training
- Work in progress

Work supported by: US DOE-NNSA Nuclear Criticality Safety Program
LANL Nuclear Criticality Safety Division
LANL PF4 Restart

MCNP Progress for NCSP

US DOE-NNSA Nuclear Criticality Safety Program –

What have we done for you lately (FY 2016, FY 2017) ?

- **Overview of LANL Analytical Methods Work for NCSP**

- **MCNP6 & Whisper Status**
- **Verification / Validation**
- **User Support & Training**

- **Work in Progress**
  - Whisper – Validation & USLs
  - Automated Convergence Diagnostic
  - MCNP 2020 – Modernization & Parallel
  - Solution Chemistry Effects on Criticality
  - Temperature Dependence
  - Correlated Fission Multiplicity

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 – 2017, with Whisper code & benchmarks

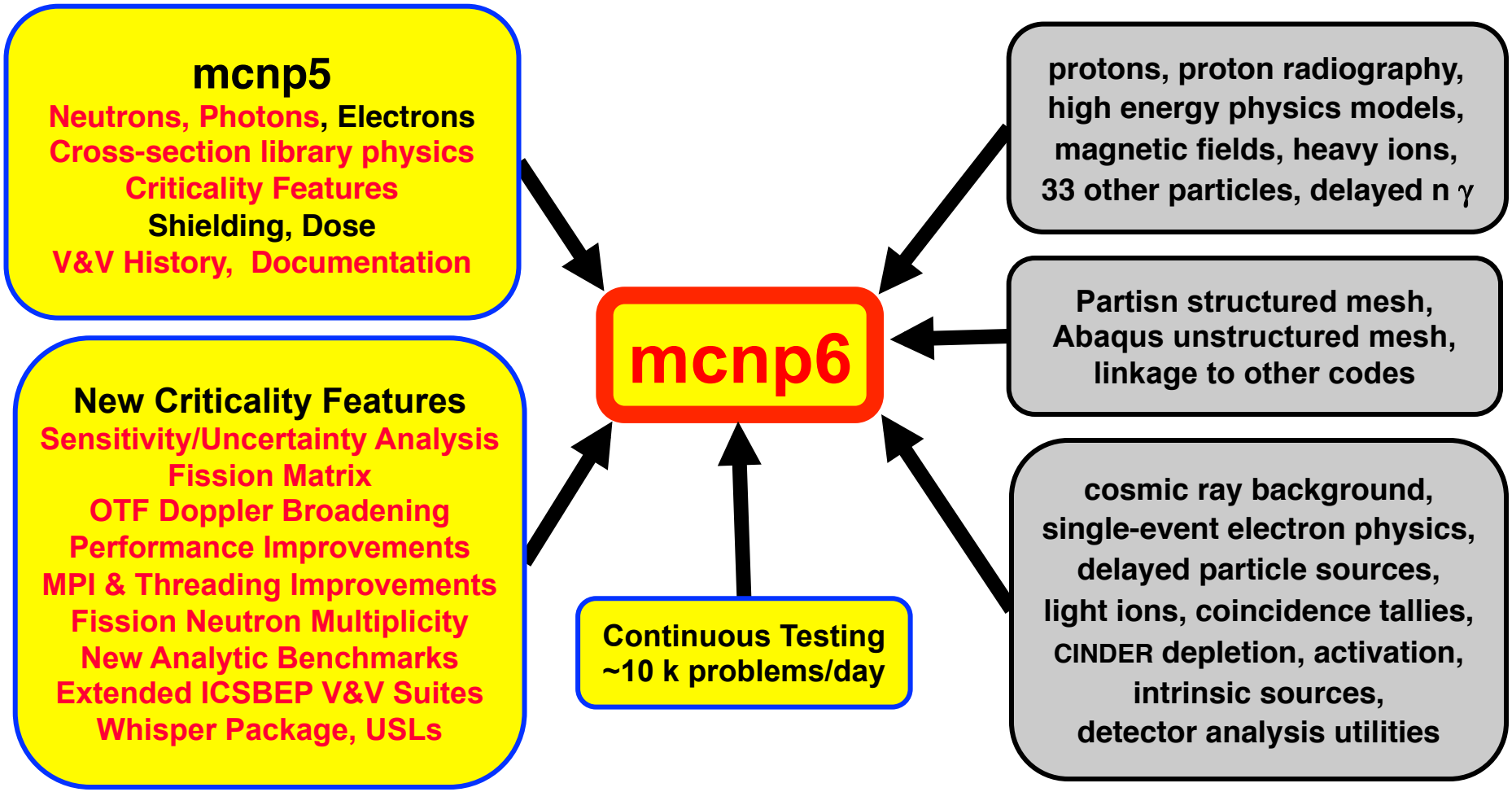
Nuclear Data – ENDF/B-VII.1 data, updates, & older data
Reference Collection – 700+ technical reports
V&V Test Collection – 1500+ test problems

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

Frequent V&V testing for NCS applications

- **Release status**
  - **In final stages of release testing & User Manual revisions**
    ~ 8,000 code files, ~ 6,000 test files, ~750 documents
  - **Extensive release-testing by MCNP Team in progress**
  - **Friendly-user testing at LANL & Sandia NCS**
  - **Expected release to RSICC: April or May 2017**

MCNP6 & Whisper Status (2)

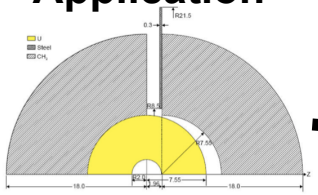


~ 2 developers

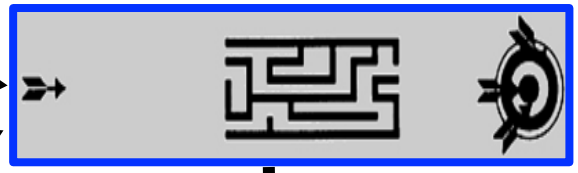
~ 8-10 developers

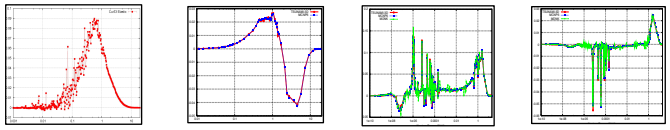
MCNP6 & Whisper Status (3)

Application



ACE Cross-section Data





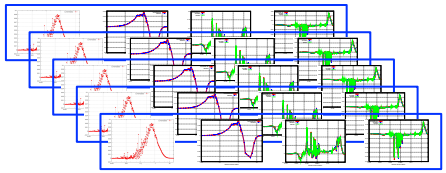
MCNP6

Monte Carlo Criticality Calculation

Application Sensitivity Profile

ACE Cross-section Covariance Data

SU-based Analysis



Catalog of sensitivity profiles for 1100+ experiments

USL

Upper Subcritical Limit for NCS analysis

Whisper

Pattern matching – application sensitivity profile vs catalog

Select similar experiments

Statistical analysis to determine bias & uncertainty & MOS

MCNP6 & Whisper Status (4)

- **MCNP6.2 new features**
  - **Same speed as MCNP6.1.1, about 2x faster than MCNP6.1**
  - **Longer input lines, up to 128 characters**
  - **Warning message regarding bias if using < 10,000 neutrons/cycle**
  - **Analytic criticality benchmarks now use continuous-energy physics**
  - **MCNPtools, ISC – next slide**
  - **Bug fixes**
    - Coincident surfaces for rotated universe/fill (25 year old bug)
    - Rare S(α,β) sampling error (due to roundoff)
    - ACE Data – hydrogen (n,γ), SiO_2 S(α,β)
    - 300+ bug-fixes since MCNP6.1, non-criticality
- **Whisper-1.1**
  - **Coding, benchmarks, scripts, & 50+ documents**
  - **Benchmark catalog - 1101 ICSBEP problems**
  - **Portable to Mac, Linux, Windows**

MCNP Utilities

- **Recent upgrades**
  - **mcnp_pstudy.pl - additional options to work with Whisper**
  - **simple_ace.pl - one-speed continuous energy cross sections**

- **New tools released (with MCNP6.2)**
  - **ISC - Intrinsic Source Constructor Library**
    - Used to generate radiation sources for transport code input (SDEF)
    - Written in C++ with Python bindings
  - **MCNPTools**
    - Library that provides object-oriented access to MCNP outputs
      - MCTAL files
      - MESHTAL B (MCNP5/FMESH) files
      - PTRAC files
    - Written in C++ with Python and Perl bindings
    - Other features also included

- **Coming soon (not with MCNP6.2)**
  - **DRiFT - Detector Response Function Toolkit**

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

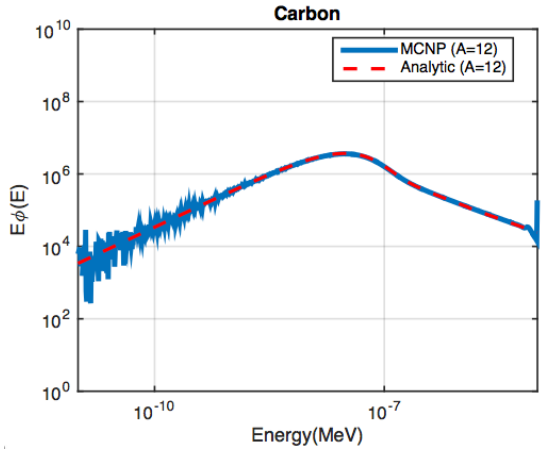
Validation Suites

- **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)

- **How accurate is MCNP6 if cross-sections & dimensions are exact?**
  - **Verification_Keff analytic suite with continuous-energy, 0-D & 1-D**
  - **37 problems run using continuous-energy, 250 M neutrons each**
  - **Results match exact analytic solutions within 0.00003 +- 0.00003**

- **Free-gas scattering benchmark (Gonzales)**
  - **Analytic benchmark for slowing down in an infinite medium, with elastic scattering – including free-gas scattering**
  - **MCNP**
    - Constant cross-sections, with Doppler broadened scattering
    - Elastic scatter with **target mass A** & **temperature T**
    - Continuous-energy elastic scatter, including target motion



User Support & Training

User Support

- **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 hands-on support for LANL NCS Division
  - Email consulting to many crit-safety analysts

- **University classes**
  - Monte Carlo class for seniors & grad students at University of New Mexico, Nuclear Eng. Dept.
  - Monte Carlo lectures for XCP Computational Physics Workshop

- **Conferences & Journals**
  - Nuc Sci Eng, Annals of Nuc En, Prog Nuc En, others
  - M&C-2015, ICNC-2015, PHYSOR-2016, M&C-2017
  - ANS …, Anaheim, San Antonio, Washington, Las Vegas, …
  - OECD Expert Groups - Advanced Monte Carlo, Sensitivity-Uncertainty

MCNP & Whisper Training

- **MCNP Classes**
  - **Theory & Practice of Criticality Calculations with MCNP (4 days)**
    - 16 theory lectures (537 slides), 18 practical lectures (780 slides), 190 examples, greatly expanded coverage of SU-methods (Whisper)
    - FY15: 3 classes (2 LANL, 1 Y-12)
    - FY16: 3 classes (2 LANL, 1 Sandia)
    - FY17: ? classes (2 LANL, ???)
- **Whisper & SU-methods Training**
  - **½-day MCNP-Whisper training module for NCS analysts**
    - Presented 2 LANL, 1 Sandia, 1 IRSN
  - **2-day Sensitivity-Uncertainty & MCNP-Whisper Training**
    - Presented at 2016 EFCOG-NFS workshop
    - MCNP-Whisper vs traditional approaches
  - **Detailed lecture notes on validation, SU methods, Whisper**
    - Informal talks at LANL, ~25 hrs, 262 slides
- **Training available for any DOE site crit-safety group, just ask**

Work in Progress

Whisper – Validation & USLs

Automated Convergence Diagnostic

MCNP 2020 – Modernization & Parallel

Solution Chemistry Effects on Criticality

Temperature Dependence

Correlated Fission Multiplicity

Other R&D Work, with Universities

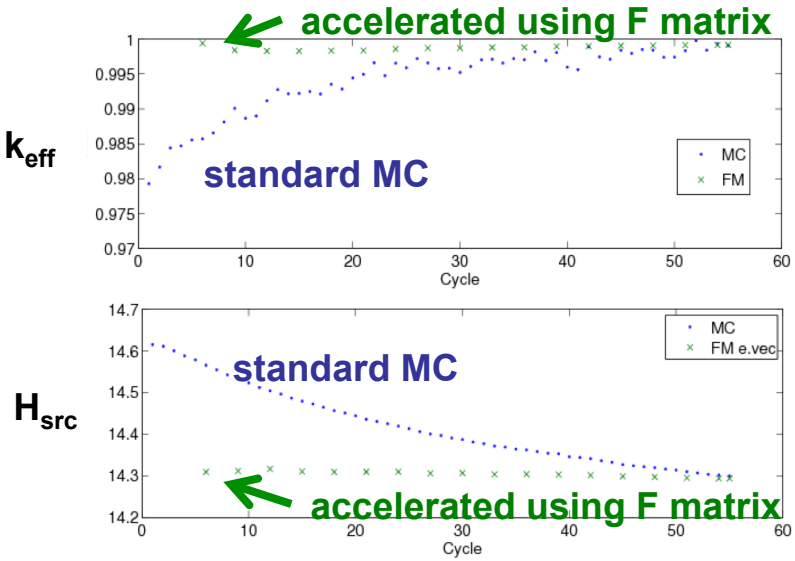
Whisper - Next Steps

- White paper on Whisper & ANS-8.24
- Expand the Whisper benchmark suite
  - Ongoing collaboration with Sandia (J Miller, S Henderson)
  - Sandia NCS has been using an early-release of Whisper during 2016
  - Exchanged benchmarks (1101 LANL, 866 Sandia)
  - Add Sandia benchmarks to Whisper catalog, ~500 new
- Investigate the impact on benchmark selection & USLs of:
  - MCNP6 statistics (noise in SU profiles)
  - Different benchmark catalogs (eg, LANL vs SNL)
  - Size & completeness of benchmark catalogs
  - Analyst or site bias? (no evidence so far)
- Improved covariance data
  - New data from Scale-6.2
  - New data from LANL, using NJOY
  - Investigate impact on benchmark selection & USLs

Automatic Convergence Diagnostic

- **History**
  - MC criticality calculations are iterative
  - Fission neutron source distribution must be converged before computing k-effective & reaction rates
  - For the first 50 years of MC criticality, no tools available to check convergence
  - 15 years ago, Ueki & Brown introduced Shannon Entropy of the fission distribution to check convergence
  - Has dramatically improved the quality & correctness of MC criticality, & now used in most MC codes worldwide
- **Today**
  - Can now diagnose convergence, but analysts are sometimes "too busy", or have not been properly educated
  - Need an automated process – code determines convergence
- **Fission matrix**
  - Discretized Green's function, region-to-region probabilities for next-gen fission
  - With fine-enough mesh for the F matrix, eigenfunction is the correct converged fission distribution

- **Fission matrix**
  - New sparse storage techniques for MCNP permit the use of very fine meshing for F, hence more accurate
  - Can determine F even if not converged
  - Can use F eigenfunction to accelerate convergence of neutron distribution
  - Can use the F eigenfunction to automatically diagnose convergence, without requiring user action



  - R&D was advanced & demo'd, but completion delayed by the importance of supporting Whisper S-U methods

MCNP 2020 – Status

MCNP 2020

- **Improve performance**
  - **Goal: 2X speedup within 2 years**
- **Upgrade core MCNP6 software**
  - **Evolution, not revolution**
  - **Restructure, clean up code & data structures, standards compliance**
  - **Reduce future costs for development & maintenance**
  - **Goal: sustainable code**
- **Prepare for future**
  - **New computers – massive parallel, but less memory per core**
  - **Improve MPI & thread parallelism**
  - **Goal: flexible, adaptable code**

MCNP 2020 - Progress:

- **2 X speedup over original MCNP6**
- **500 k lines of code are now 100% compliant with Fortran-2003 standard**
- **Test MCNP6 on Intel Phi (MIC)**
  - No changes needed in source coding
  - Works with 100s of threads
  - Needs some tuning
- **Code infrastructure**
  - Transitioned to GIT for version control
  - Consolidated I/O files
  - Memory allocation in progress
- **Parallel threading**
  - Enhancements in progress
- **New compilers**
  - Intel-15, Intel-16, Intel-17
  - gfortran-5.3, gfortran-6.2

MCNP 2020 - Performance Improvements

Run Times for VALIDATION_CRITICALITY Suite on Various Computers

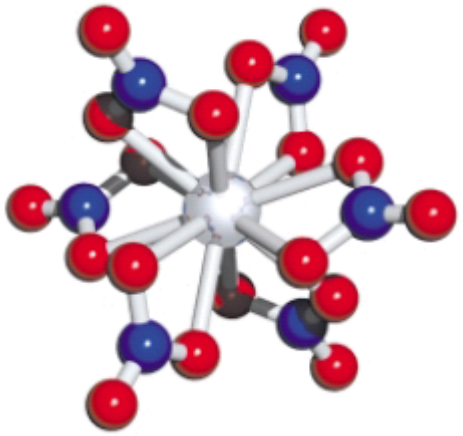
Computer	CPU Speed (GHz)	Mem. Speed (GHz)	Processors, Cores, Hyperthreads	MCNP Threads used	MCNP Version	Total Time (minutes)	
MacBook 2010	2.7	1.1	1 - i7, 2 x 2 HT	4	mcnp6.1.1	88	
MacBook 2013	3.0	1.6	1 - i7, 2 x 2 HT	4	mcnp6.1	62	
				4	mcnp6.1.1	42	
Mac Pro 2010	3.0	0.67	2 - Xeon, 4	8	mcnp6.1	44	
				8	mcnp6.1.1	28	
Windows 2012	2.7	1.3	2 - Xeon, 6	10	mcnp6.1.1	19	
Mac Pro 2012	2.4	1.07	2 - Xeon, 4 x 2 HT	16	mcnp6.1.1	22	
Mac Pro 2014	2.7	1.6	1 - Xeon, 12 x 2 HT	12	mcnp5-1.60	14	
				12	mcnp6.1.1	14	
				12	mcnp6.2	12	←
HP Linux 2015	2.6	2.1	2 - Xeon, 8	16	mcnp6.2	10	
HP Linux 2016	3.1	2.4	2 - Xeon, 12 x 2 HT	24	mcnp6.2	8	
HP Linux 2017	2.1	2.4	2 - Xeon, 18 x 2 HT	36	mcnp6.2	6½	←

MCNP6.2 preserves all performance improvements from MCNP6.1.1, and is much faster than MCNP6.1 & slightly faster than MCNP5

Runtimes are wall-clock for the entire suite of 31 problems, including cross-section I/O & output

Solution Chemistry Effects on Criticality

- **Investigating Impact of Chemistry in Modeling Plutonium Solution**
  - **Oxidation state**
    - Pu(III), Pu(IV), Pu(V), Pu(VI), Pu(VII) exist in solution
    - Pu(III), Pu(IV), Pu(V) and Pu(VI) can exist simultaneously in acid
  - **Speciation/Coordination Chemistry**
    - In Pu(IV) nitrate solutions
      - $Pu(NO_3)_2^{2+}$ highest concentration in 2 M nitric acid
      - $Pu(NO_3)_4$ and $Pu(NO_3)_6^{2-}$ in 7 M nitric acid
      - $Pu(NO_3)_6^{2-}$ highest concentration in 13 M nitric acid
  - **Density**
  - **Effects of Temperature**
    - Influences disproportionation and density
  - **Effects of Radiolysis**
    - Influences disproportionation
  - **Whisper methodology to characterize neutronics**
    - Used to compare neutronics of solution system with different ligands
    - Investigations comparing plutonium chloride solutions with nitrate solutions



$Pu(NO_3)_6^{2-}$
Los Alamos Science Number 26. 2000.

Temperature Dependence

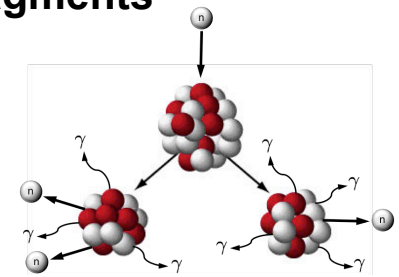
- **Nearly all NCS calculations are done at room temperature**
- **For hot or cold calculations:**
  - **Material densities & problem dimensions are affected by temperature**
  - **Neutron physics is affected by temperature:**
    - Doppler broadening of resonance cross-sections
    - Changes in thermal scattering due to temperature effect on nuclide motion
    - Changes in epithermal scattering due to temperature effect on nuclide motion
  - **In principle, can use NJOY & MCNP with different temperatures, but can be very tedious & error-prone**

- **Over the past years, R&D was completed with 4 PhD students on new methods for continuous variation in temperature in MCNP calculations**
  - **On-the-fly Doppler broadening**
    - Gokhan Yesilyurt (Michigan) thesis
    - Already in MCNP6
  - **On-the-fly S(a,b) temperature**
    - Andrew Pavlou (RPI) thesis
    - Demo'd in MCNP6
  - **On-the-fly unresolved resonances**
    - Jonathan Walsh (MIT) thesis
    - Demo'd in OpenMC code
  - **DBRC**
    - Doppler broadening resonance correction for epithermal scatter
    - Eva Sunny (Michigan) thesis
    - Demo'd in MCNP5
- **These can all be made permanent features in MCNP6**

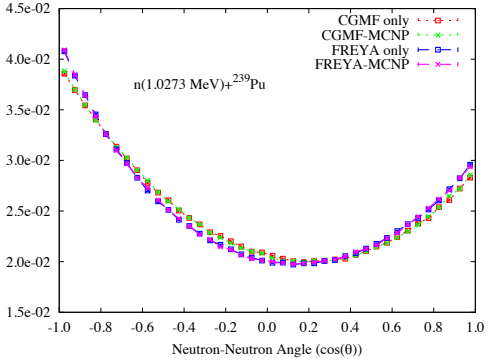
Correlated Fission Multiplicity

Secondary Emission from Fission

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

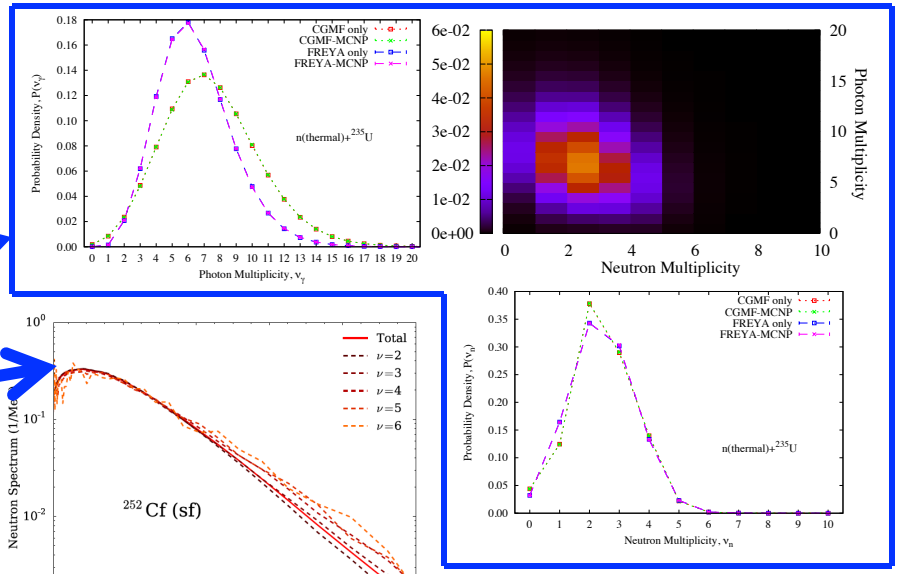


- Multiplicity distribution of neutrons and gamma rays
- Multiplicity-dependent energy spectra
- Angular emission from fission fragments



What's New in MCNP6.2

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



- Not available for criticality calculations yet… (UNM student thesis work)

Summary

- **MCNP releases**
  - **MCNP5 is no longer supported, cannot use continuous S(a,b)**
  - **MCNP6.1, MCNP6.1.1, & ENDF/B-VII.1 released in 2013 & 2014**
  - **MCNP6.2 & Whisper release – April/May 2017**
    - 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
- **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, code maintenance, training**
- **Work in progress – 6 major areas**
  - **Whisper, S-U methods**
  - **Automated convergence diagnostic**
  - **MCNP 2020 modernization & parallel improvements**
  - **Solution chemistry effects**
  - **Temperature effects**
  - **Correlated fission multiplicity**

Questions ?