MCNP Progress for the Nuclear Criticality Safety Program

LA-UR-16-28500

Forrest Brown, Michael Rising, Jennifer Alwin

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

Abstract

MCNP Progress for the Nuclear Criticality Safety Program

Forrest Brown, Michael Rising, Jennifer Alwin

Monte Carlo Methods, Codes, & Applications, LANL

The DOE/NNSA Nuclear Criticality Safety Program (NCSP) supports research, development, maintenance, and verification and validation of the MCNP Monte Carlo radiation transport software package 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 2015 and early FY 2016. Activities and accomplishments are summarized in five major areas:

- **MCNP6 status,**
- **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 2015, FY 2016) ?

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

MCNP6 Status

MCNP6 Status (1)

- **MCNP releases by RSICC**

MCNP5	– 2003-2013, R.I.P.
MCNP6.1	– 2013, production version
MCNP6.1.1	– 2014, same criticality, faster, beta features for DHS
MCNP6.2	– 2017, will include 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

12,000^{+} copies of MCNP5 distributed by RSICC

8,000^{+} copies of MCNP6 distributed by RSICC

- **MCNP6 usage on HPC systems at LANL**
  - MCNP6 is used for about 1,000,000 hours / month.
  - Criticality safety accounts for 10-20% of usage.

MCNP6 Status (2)

mcnp5
Neutrons, Photons, Electrons
Cross-section library physics
Criticality Features
Shielding, Dose
V&V History, Documentation

New Criticality Features
Sensitivity/Uncertainty Analysis
Fission Matrix
OTF Doppler Broadening
Performance Improvements
MPI & Threading Improvements
Fission Neutron Multiplicity
New Analytic Benchmarks
Extended ICSBEP V&V Suites
Whisper Package, USLs

mcnp6

Continuous Testing
~10 k problems/day

mcnp6
protons, proton radiography
high energy physics models
magnetic fields

Partisn structured mesh
Abaqus unstructured mesh

mcnpx
33 other particles, heavy ions
CINDER depletion, delayed n γ

High energy physics models
CEM, LAQGSM, LAHET, MARS, HETC
cosmic ray background
Single-event electron physics
delayed particle sources
coincidence tallies

mcnp5 – 100 K lines of code
mcnp6 – 500 K lines of code

MCNP6.2 Release to RSICC

- **MCNP6.2 new features**
  - **Longer input lines, up to 128 characters**
  - **Longer command-line, to support 256-character filenames**
  - **Bug fixes**
    - Coincident surfaces for rotated universe/fill (25 year old bug)
    - Rare S(alpha,beta) sampling error (due to roundoff)
  - **Features for criticality**
    - Analytic criticality benchmarks now use continuous-energy physics
    - Warning message regarding bias if using < 10,000 neutrons/cycle
    - Same performance (speed) as MCNP6.1.1 (2x MCNP6.1)
    - **Whisper** coding, benchmarks, scripts, & documentation
  - **Many other bug fixes & features, for non-criticality problems**

- **Release status**
  - **In final stages of code reviews, feature reviews, & clean up**
  - **Final documentation, release testing, & installers soon**
  - **Expected release to RSICC: late-2016 or early 2017**

Whisper Status

Whisper Methodology for Validation & USLs

- **In early 2014, the XCP-3 & NCS groups at LANL undertook a major upgrade to the criticality safety computational capabilities**

  MCNP6.1 + ENDF/B-VII.1 + Whisper-1.0 + ICSBEP + HPC cluster

- **Whisper-1.1 – 2016**
  - Benchmark catalog expanded to 1101 ICSBEP, with a few corrections
  - New scripts, portable to Linux, Mac, & Windows
  - Whisper coding – portability mods (no bug fixes needed)

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

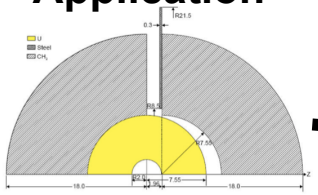
  ① Automated, physics-based selection of benchmarks that are neutronically similar to the application, ranked & weighted

  ② Bias + bias uncertainty from Extreme Value Theory

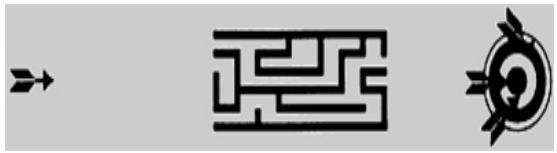
  ③ Margin for nuclear data uncertainty estimated by GLLS method

MCNP-Whisper Methodology for NCS Validation

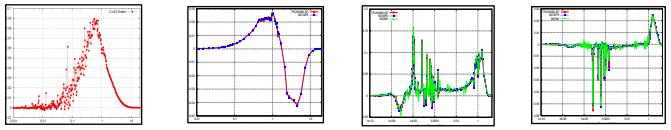
Application



Nuclear Cross-section Data



MCNP6
Monte Carlo Criticality Calculation



Application Sensitivity Profile

Nuclear Cross-section Covariance Data

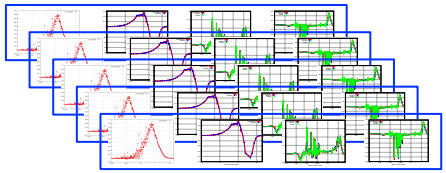
SU-based Analysis

Whisper

Pattern matching – application sensitivity profile vs catalog

Select similar experiments

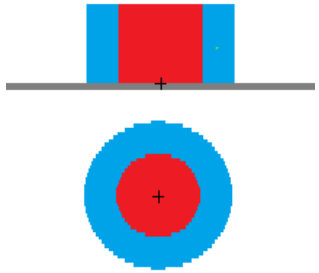
Statistical analysis to determine bias & uncertainty & MOS



Catalog of sensitivity profiles for 1100+ experiments

USL
Upper Subcritical Limit for NCS analysis

Example: Pu cylinder, H/D=1, water reflector, steel floor



```
Calculating application nuclear data uncertainties ...
   application                                    adjusted    prior
   pu-hd-1.0                                      0.00075     0.01385

Calculating upper subcritical limits ...
                                                  calc        data unc    baseline
   application                                    margin      (1-sigma)   USL
   pu-hd-1.0                                      0.01443     0.00075     0.97863

   Benchmark population     =   43
   Population weight        =  25.30973
   Maximum similarity       =   0.99691

   Bias                     =   0.00850
   Bias uncertainty         =   0.00593
   Nuc Data uncert margin   =   0.00075
   Software/method margin   =   0.00500
   Non-coverage penalty     =   0.00000

   benchmark                                      ck          weight
   pu-met-fast-036-001.i                          0.9969      1.0000
   pu-met-fast-024-001.i                          0.9966      0.9916
   pu-met-fast-022-001.i                          0.9948      0.9386
   pu-met-fast-023-001.i                          0.9931      0.8887
   pu-met-fast-044-005.i                          0.9931      0.8870
   . . . . . . . . . .
   mix-met-fast-007-022.i                         0.9724      0.2824
   mix-met-fast-007-023.i                         0.9693      0.1915
   pu-met-fast-045-005.i                          0.9670      0.1240
   pu-met-fast-003-103.i                          0.9662      0.1021
   mix-met-fast-001-001.i                         0.9650      0.0664
```

For this application, 43 of the 1101 benchmarks were selected as neutronically similar & sufficient for valid statistical analysis

Benchmark rankings shown below

Excellent c_k's In range .96 - .99

Traditional validation gave USL = 0.970

NCS & Validation

- **No one is suggesting that traditional validation methods should be scrapped & replaced by sensitivity-uncertainty methods**
- **One of the most important parts of traditional validation is picking a set of benchmark experiments that are similar to your work**
  - **In the past this was based solely on "expert judgment"**
    - Not repeatable, difficult to justify when audited. What if no experts?
- **Sensitivity-uncertainty tools are now available, from ORNL & LANL**
  - **Can provide quantitative, repeatable, physics-based evidence that the set of benchmarks is appropriate**
  - **Can provide additional justification for oddball cases where no similar benchmarks exist**
  - **Can provide guidance & starting point for determining extra MOS for data, codes, applicability**
- **It's time for NCS analysts to learn about SU-based methods & begin to incorporate them into the validation process**
- **The next 5 years should be a transition period, using both traditional & SU methods for validation**

Verification
&
Validation

MCNP Verification & Validation

See other papers at this meeting:
Brown & Rising, Verification of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for Criticality Safety Applications
Brown, New Version of the MCNP Analytic Criticality Benchmark Suite

Verification Suites

- **REGRESSION**
  - 161 code test problems
  - Run by developers for QA checking
- **VERIFICATION_KEFF**
  - 75 analytic benchmarks (0-D and 1-D)
  - Exact solutions for k_{eff}
  - Past – multigroup,
    New – continuous-energy
- **VERIFICATION_GENTIME**
  - 10 benchmarks (analytic or comparisons to Partisn) for reactor kinetics parameters
- **KOBAYASHI**
  - 6 void & duct streaming problems, with point detectors, exact solutions
- **Ganapol Benchmarks** [in progress]
  - Exact, semi-analytic benchmark problems
  - Fixed source, not criticality
- **Gonzales Benchmark** [in progress]
  - Exact analytic benchmark with elastic scatter, including free-gas scatter

Validation Suites

- **VALIDATION_CRITICALITY**
  - 31 ICSBEP Cases
  - Too small a suite for serious V&V
  - Today, used for
    - Code-to-code verification, with real problems & data
    - Compiler-to-compiler verification, with real problems & data
    - Timing tests for optimizing MCNP coding & threading
- **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

MCNP6 Criticality Verification

How accurate is MCNP6 if cross-sections & dimensions are exact ?

Verification_Keff

- **A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code Verification", *Prog. Nucl. Energy*, 42, 55-106 (2003). Also, LA-UR-01-3082, from mcnp.lanl.gov**
- **Compilation of 75 criticality problems from the literature with <u>exact</u> analytic solutions**
- **Complete overhaul in the past months**
  - Utilities to construct ACE files, multigroup & continuous-energy
  - Revised & checked xsecs & geometry (more digits in input, …..)
- **First time ever that this suite has been run using the continuous-energy physics routines in MCNP (previously, multigroup only)**
- **37 problems run using continuous-energy, 250 M neutrons each**
- **Results match exact analytic solutions within 0.00003 +- 0.00003**

MCNP6 Criticality Results vs Exact Results

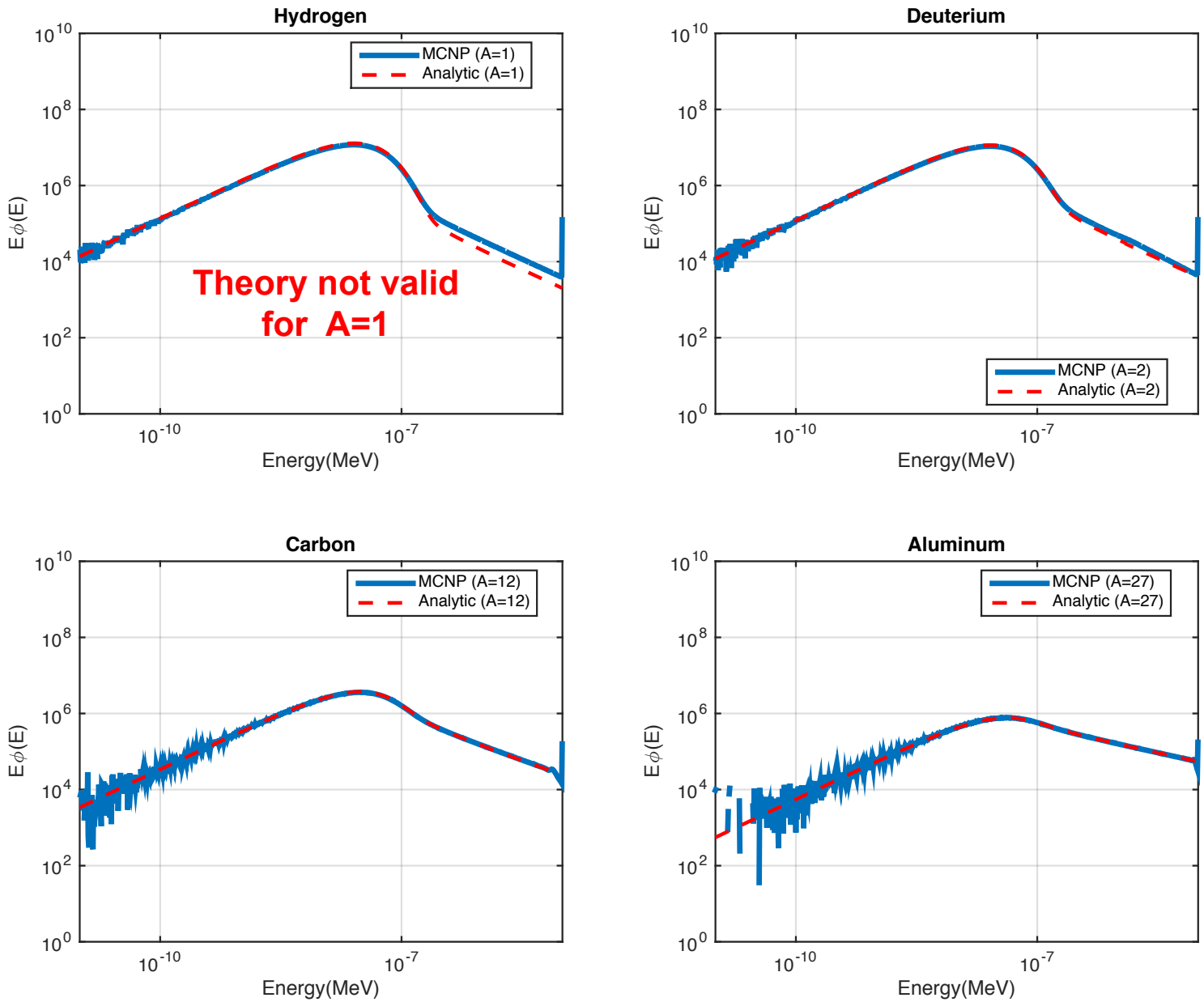
Case	Name	Analytic keff	MCNP_Multigroup C/E-1	std	MCNP Continuous Energy C/E-1	std
01	PUa-1-0-IN	2.61290	-0 pcm	0	-0 pcm	0
02	PUa-1-0-SL	1.00000	0	5	6	5
03	PUa-H2O(1)-1-0-SL	1.00000	8	5 *	1	5
04	PUa-H2O(0.5)-1-0-SL	1.00000	2	5	3	5
05	PUb-1-0-IN	2.29032	-0	0	-0	0
06	PUb-1-0-SL	1.00000	4	4	0	4
07	PUb-1-0-CY	1.00000	-4	4 *	3	4
08	PUb-1-0-SP	1.00000	6	4 *	6	4 *
09	PUb-H2O(1)-1-0-CY	1.00000	-3	4	5	4
10	PUb-H2O(10)-1-0-CY	1.00000	5	4	5	5
11	Ua-1-0-IN	2.25000	0	0	0	0
12	Ua-1-0-SL	1.00000	6	4 *	-3	4
13	Ua-1-0-CY	1.00000	4	4	3	4
14	Ua-1-0-SP	1.00000	1	4	-5	4 *
15	Ub-1-0-IN	2.33092	0	0	0	0
16	Ub-H2O(1)-1-0-SP	1.00000	-2	4	-1	4
17	Uc-1-0-IN	2.25608	0	0	0	0
18	Uc-H2O(2)-1-0-SP	1.00000	-1	4	0	4
19	Ud-1-0-IN	2.23267	-0	0	-0	0
20	Ud-H2O(3)-1-0-SP	1.00000	4	4	7	4 *
21	UD2O-1-0-IN	1.13333	-0	0	-0	0
22	UD2O-1-0-SL	1.00000	3	2	0	2
23	UD2O-1-0-CY	1.00000	-1	2	-5	2 **
24	UD2O-1-0-SP	1.00000	1	3	-4	2 **
25	UD2O-H2O(1)-1-0-SL	1.00000	2	2	-2	2 *
26	UD2O-H2O(10)-1-0-SL	1.00000	-5	2 **	1	2
27	UD2O-H2O(1)-1-0-CY	1.00000	4	2 *	-1	2
28	UD2O-H2O(10)-1-0-CY	1.00000	0	2	3	2
29	Ue-1-0-IN	2.18067	0	0	0	0
30	Ue-Fe-Na-1-0-SL	1.00000	-1	5	7	4 *
31	PU-1-1-IN	2.50000	0	0	0	0
32	PUa-1-1-SL	1.00000	8	5 *	7	5 *
36	Ua-1-1-CY	1.00000	2	4	-3	4
38	UD2Oa-1-1-IN	1.20559	0	0	0	0
39	UD2Oa-1-1-SP	1.00000	-2	3	2	3
40	UD2Ob-1-1-IN	1.22739	-0	0	-0	0
41	UD2Ob-1-1-SP	1.00000	8	3 **	6	3 *
		RMS Differences	3 pcm	±3 pcm	3 pcm	±3 pcm

1 pcm = 0.00001

Gonzales Benchmark

- **Gonzales, Prinja, Brown, Kiedrowski, "An Analytic Benchmark of Neutron Free-gas Scattering Using Continuous-energy Cross Sections in MCNP6", PHYSOR 2016, Sun Valley, Idaho, LA-UR-15-26797**
- **Gonzales, Prinja, Kiedrowski, Brown, "Piecewise Constant Heavy Gas Model for Free-Gas Elastic Scattering", this meeting**
  - **Analytic benchmark for slowing down in an infinite medium, with elastic scattering – including free-gas scattering**
  - **First analytic benchmark (ever) to address free-gas scattering**
  - **Based on exact solution using heavy-gas model**
    - Does not apply for A=1
    - For large A, approaches correct solution
  - **MCNP**
    - Constant cross-sections
    - Elastic scatter with **target mass A** & **temperature T**
    - Continuous-energy elastic scatter, including target motion

Gonzales Benchmark – for Various A



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. each Fall
  - Monte Carlo lectures for XCP Computational Physics Workshop each summer

- **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)
    - FY14: 3 classes (2 LANL, 1 Hanford)
    - FY15: 3 classes (2 LANL, 1 Y-12)
    - FY16: 3 classes (2 LANL, 1 Sandia)

- **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**

Work in Progress

Whisper – Validation & USLs

MCNP 2020 – Status

Other R&D Work, with Universities

Whisper - Next Steps

- **Prepare Whisper for MCNP6.2 distribution**
- **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)**
  - **356 benchmarks were common to both LANL & SNL suites**
    - Ave. bias for LANL cases = 0.00175 +- 0.00024
    - Ave. bias for SNL cases = 0.00179 +- 0.00021
    - Average SNL-LANL diff = 0.00004 +- 0.00010
- **Investigating the impact of MCNP6 statistics (noise in SU profiles) on Whisper USLs**
- **Investigating the impact of different benchmark catalogs**
  - **Compare Whisper USLs using LANL & Sandia catalogs**
  - **Randomly eliminate 10%, 20%, or 50% of catalog, see effect on USL**
- **White paper on Whisper & ANS-8.24**

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	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
				14	mcnp6.1.1	12
				14	mcnp6.2	12
HP Linux 2016	3.1	2.4	2 - Xeon, 12 x 2 HT	24	mcnp6.2	8

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

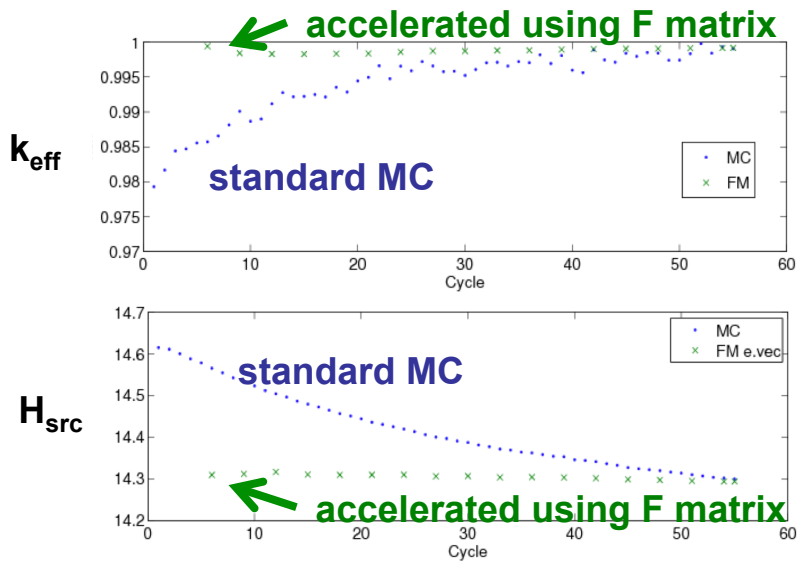
Other R&D work, with Universities

Physics & Temperature Dependence

- Full temperature dependence of S(a,b) thermal scattering (RPI)
- Unresolved resonances (MIT)
- Implement modified free-gas scatter, to model resonance upscattering for epithermal neutrons (Michigan)
- V&V for using explicit fission neutron multiplicity distributions in criticality calculations (New Mexico)
- Doppler coefficients & analytic benchmarks (New Mexico)

Fission Matrix

- Forward & adjoint methods, sparse matrix schemes (Michigan)
- Automatically determine source convergence, without user input
- Accelerate source convergence



Summary

- MCNP6.1, MCNP6.1.1, & ENDF/B-VII.1 released in 2013 & 2014
- MCNP6.2 & Whisper release – late 2016 or early 2017

- Impact on Criticality Calculations ➜ none
  - All basic KCODE criticality features same as for MCNP5 & MCNP6.1
  - Matches results with MCNP5 for criticality suites (for same compiler)

- MCNP6 speed improved by 1.2 – 4 X for crit-safety.
- More MCNP 2020 improvements in progress

- Sensitivity-uncertainty methods based on adjoint-weighted tallies are being used routinely in many areas
  - Outstanding success due to long-range vision & support from NCSP

- Whisper methodology for validation & USLs is important to LANL NCS, and to other DOE sites. Training is available.

- Criticality-safety community needs to transition to MCNP6.
  - MCNP5 is no longer supported, cannot use continuous S(a,b)

Questions ?

LA-UR-16-28500
Approved for public release; distribution is unlimited.

Title: MCNP Progress for the Nuclear Criticality Safety Program

Author(s): Brown, Forrest
Rising, Michael
Alwin, Jennifer

Intended for: ANS 2016 Winter Meeting
Las Vegas, NV

Issued: 2016-11-06