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Title: **MCNP Progress for NCSP**

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Technical Program Review
15-16 March 2016

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MCNP Progress for NCSP

Forrest Brown, Michael Rising, Jennifer Alwin
Monte Carlo Codes, XCP-3
Los Alamos National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

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)

Monte Carlo Codes
XCP-3, LANL

- **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 – 2016 (?), will include Whisper code & benchmarks

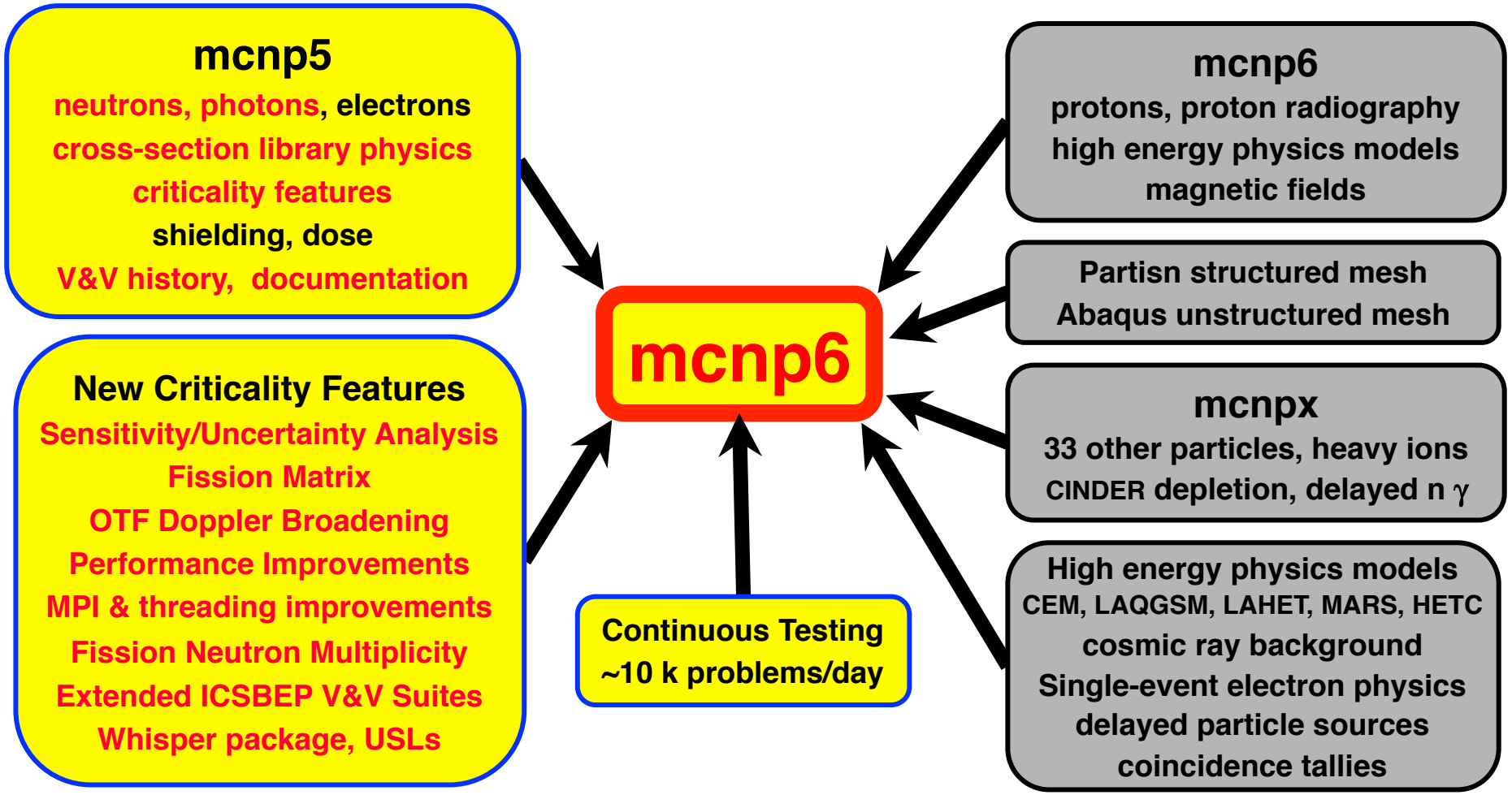
  Nuclear Data – ENDF/B-VII.1 data, updates, & older data
  Reference Collection – 700+ technical reports
  V&V Test Collection – 1434 test problems

  12,000+ copies of MCNP5 distributed by RSICC
  8,000+ copies of MCNP6 distributed by RSICC

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

MCNP6 Status (2)

Monte Carlo Codes
XCP-3, LANL



mcnp5 – 100 K lines of code

mcnp6 – 500 K lines of code

Whisper
Status

Whisper? Who cares?

- Sensitivity/Uncertainty methods for validation have been under development for > 18 yrs at ORNL (Broadhead, Rearden, Perfetti, ...)
- Kiedrowski & Brown developed MCNP iterated fission probability, adjoint weighted tallies, & S/U capabilities, 2008-2013. Whisper in 2014.
- There are now 2 calculational paths for S/U based validation:
  - SCALE/Tsunami/Tsurfer
  - MCNP/Whisper
- International effort for comparisons being planned
  - LANL, ORNL, IRSN
- S/U based validation methods can supplement, support, & extend traditional validation methods

Whisper Methodology for Validation & USLs

Monte Carlo Codes XCP-3, LANL

- **In early 2014, the XCP-3 & NCS groups at LANL undertook a major upgrade to the criticality safety computational capabilities**
  - **Previous: mcnp5-1.25, endf 4, 5, 6 (very old, unsupported)**
  - **Upgrade: mcnp6.1 + endf/b-vii.1, whisper, HPC cluster**
  - **Participants:**
    - Kiedrowski, Conlin, Favorite, Kahler, Kersting, Parsons, Walker, Brown, etc.
- **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

Whisper Status

Monte Carlo Codes
XCP-3, LANL

- **Whisper SQA**
  - **Whisper is now part of MCNP6, rigorous SQA**
  - **Portable to Linux & Mac (Windows soon), same results**

- **Whisper Benchmark Suite**
  - **1101 ICSBEP benchmarks from Mosteller, Kahler, LANL NCS, others**
  - **For each benchmark, sensitivity profiles from MCNP6 are available for all isotopes & all reactions**
  - **Whisper can be used to identify inconsistent benchmarks (outliers)**
  - **Whisper can be used to fill-in missing benchmark uncertainties**

  - **The Whisper benchmark suite is available now to anyone, on request**
    - Already sent to Y-12, Sandia, Savannah River, ANL, & a consultant

- **Whisper software**
  - **Available to any DOE crit-safety group in FY 2016 Q3**
  - **Will be included with MCNP6.2 release (Fall 2016?)**

Whisper Documentation

Monte Carlo Codes
XCP-3, LANL

THEORY

B.C. Kiedrowski, F.B. Brown, et al., "Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits", Nuc. Sci. Eng. Sept. 2015, LA-UR-14-26558 (2014),

B.C. Kiedrowski, "Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation", LA-UR-14-23202 (2014)

F.B. Brown, M.E. Rising, J.L. Alwin, "Lecture Notes on Criticality Safety Validation Using MCNP & Whisper", LA-UR-16-21659 (2016)

USER MANUAL

B.C. Kiedrowski, "User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation", LA-UR-14-26436 (2014)

APPLICATION

B.C. Kiedrowski, et al., "Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems", LA-UR-14-23352 (2014)

SOFTWARE QUALITY ASSURANCE

R.F. Sartor, F.B. Brown, "Whisper Program Suite Validation and Verification Report", LA-UR-15-23972 (2015-05-28)

R.F. Sartor, F.B. Brown, "Whisper Source Code Inspection Report", LA-UR-15-23986 (2015-05-28)

R.F. Sartor, B.A. Greenfield, F.B. Brown, "MCNP6 Criticality Calculations Verification and Validation Report", LA-UR-15-23266 (2015-04-30)

Monte Carlo Codes Group (XCP-3), "Whisper - Software for Sensitivity-Uncertainty-based Nuclear Criticality Safety Validation", LANL TeamForge Tracker system, Artifact artf36407 (2015)

Monte Carlo Codes Group (XCP-3), WHISPER module in LANL TeamForge GIT repository (2015)

Monte Carlo Codes Group (XCP-3), MCNP6 module in LANL TeamForge GIT repository

Monte Carlo Codes Group (XCP-3), "MCNP Process Documents", LANL Teamforge wiki for MCNP

Monte Carlo Codes Group (XCP-3), "Software Quality Assurance", LANL Teamforge wiki for MCNP, P1040-rev9 requirements

Whisper Training

Monte Carlo Codes
XCP-3, LANL

- **LANL NCS training + 2016 EFCOG-NFS**
  - **Analyst training module for Whisper [in preparation]**
  - **2016 EFCOG-NFS workshop**
    - MCNP/Whisper & Scale/Tsunami vs traditional approaches
    - James Kuropatwinski (LANL-NCS) is organizer
  - **Both require basically the same approach for Whisper**
  - **Sandia crit-safety also interested in participating**

- **Demo for training (1/2 day):**
  - **Portable PC / Mac / Linux version**
    - Whisper executable – note that it should not be export controlled
    - User scripts – converted to perl, for portability
  - **Medium-sized set of benchmarks for demo**
    - Should choose enough so that validation could be done “old” & “new”
  - **A few typical application problems**
  - **Slides for hands-on demo**
  - **Computers**
    - At LANL: MCNP6 + Whisper
    - Elsewhere: Whisper only, due to time, complexity, & export control

Outline of Training Module

Whisper training, ½ day session (March?):

- Brief review of validation & USLs for NCS
- Brief review of MCNP6 sensitivity/uncertainty features & Whisper statistical analysis
- Use of the whisper_mcnp script to obtain MCNP6 sensitivity profiles for an application
- Use of the whisper_usl script to obtain the Whisper baseline USL for an application
- Case studies – 2-3 examples with specific models from recent work
- whisper_mcnp input, detailed review of MCNP6 output & sensitivity profiles
- whisper_usl input, detailed review of Whisper output & baseline USL
- Discussion, including comparison to traditional validation approach

In addition, a 1-2 hr follow-up session could be held later, to address questions that arise after NCS analysts have gained experience with Whisper over a few weeks or months.

Whisper Demo

Monte Carlo Codes
XCP-3, LANL

```
Calculating application nuclear data uncertainties ...
    application                                adjusted    prior
    in-28-2-1.txt                              0.00209     0.01221

 Calculating upper subcritical limits ...
                                               calc        data unc    baseline    k(calc)
    application                                margin      (1-sigma)   USL         > USL
    in-28-2-1.txt                              0.01334     0.00209     0.97623    -0.00686

    Benchmark population    =   48
    Population weight       =  28.56732
    Maximum similarity      =   0.96434

    Bias                    =   0.00850
    Bias uncertainty        =   0.00484
    Nuc Data uncert margin  =   0.00209
    Software/method margin  =   0.00500
    Non-coverage penalty    =   0.00000

    benchmark                                  ck          weight
    pu-met-fast-011-001.i                      0.9643      1.0000
    pu-met-fast-044-002.i                      0.9641      0.9958
    pu-met-fast-021-002.i                      0.9618      0.9545
    pu-met-fast-003-103.i                      0.9602      0.9252
    pu-met-fast-026-001.i                      0.9594      0.9099
    pu-met-fast-025-001.i                      0.9584      0.8912
    pu-met-fast-032-001.i                      0.9572      0.8699
    pu-met-fast-016-001.i                      0.9546      0.8221
    pu-met-fast-027-001.i                      0.9546      0.8217
                        .........
    pu-met-fast-012-001.i                      0.9167      0.1283
    pu-met-fast-040-001.i                      0.9166      0.1269
    pu-met-fast-045-003.i                      0.9163      0.1209
    pu-met-fast-045-004.i                      0.9147      0.0909
    pu-met-fast-002-001.i                      0.9145      0.0874
```

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

Benchmark rankings shown below

Comments & Discussion

Traditional validation methods are 40+ years old; S/U methods are new

Should not argue for exclusive use of either traditional or S/U methods

The foundation of criticality safety includes conservatism, continuous improvement, state-of-the-art tools & data, thorough checking, …..

Traditional & S/U methods complement each other, & provide greater assurance for setting USLs

- **Traditional methods provide a check on S/U methods**
- **S/U approach to automated benchmark selection is quantitative, physics-based, & repeatable. Provides a check on traditional selection**
- **Traditional methods use $MOS_{data+code}$ of 2-5%.**
  Quantitative, physics-based, repeatable $MOS_{data+code}$ from S/U usually smaller

The next 5 years or so should be a transition period, where both traditional & S/U methods should be used

In today's environment of audits, reviews, & "justify everything", it is prudent to use both traditional & S/U methods for validation

Verification
&
Validation

MCNP Verification & Validation Suites

Monte Carlo Codes
XCP-3, LANL

Verification Suites

- **REGRESSION**
  - 161 code test problems
  - Run by developers for QA checking (100s of times per day)
- **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

How accurate is MCNP6 if cross-section data & physics 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 exact 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 Results vs Exact Results

Monte Carlo Codes
XCP-3, LANL

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			

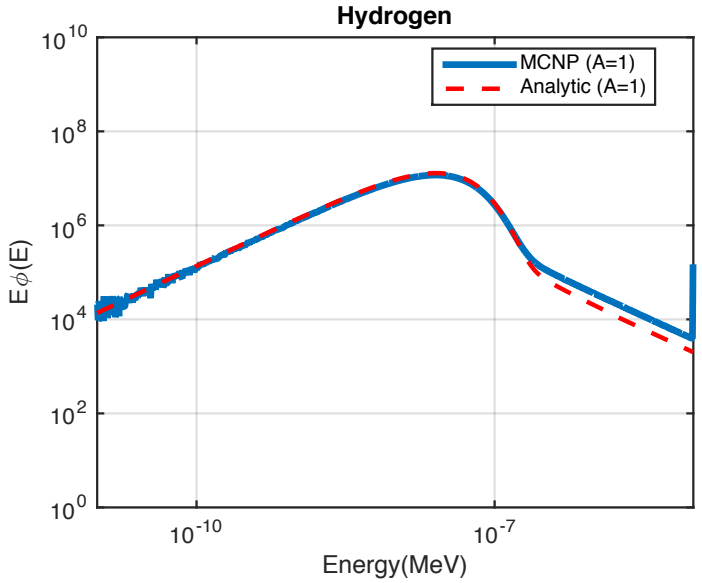
1 pcm = 0.00001

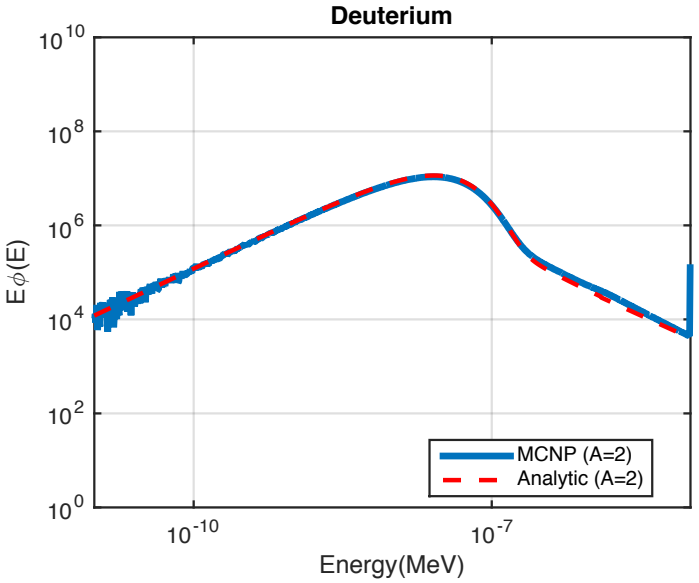
Gonzales Benchmark

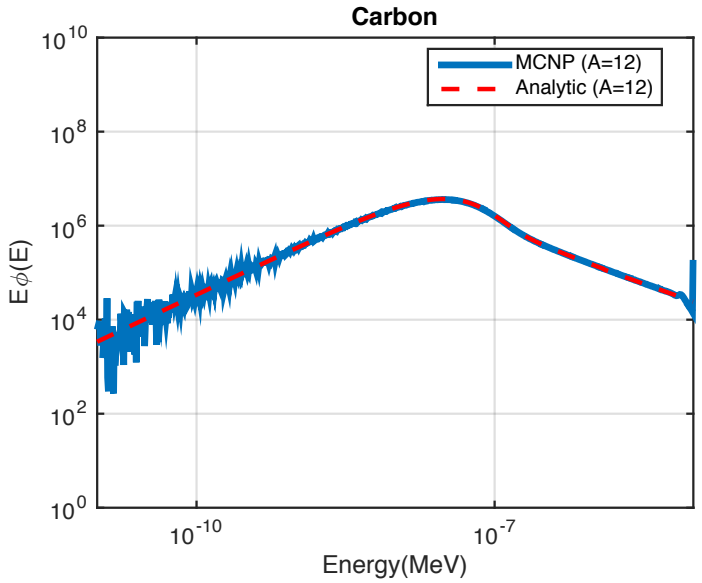
- **Matthew Gonzales, Anil Prinja, Forrest Brown, Brian Kiedrowski, "An Analytic Benchmark of Neutron Free-gas Scattering Using Continuous-energy Cross Sections in MCNP6", PHYSOR 2016, Sun Valley, Idaho, LA-UR-15-26797**

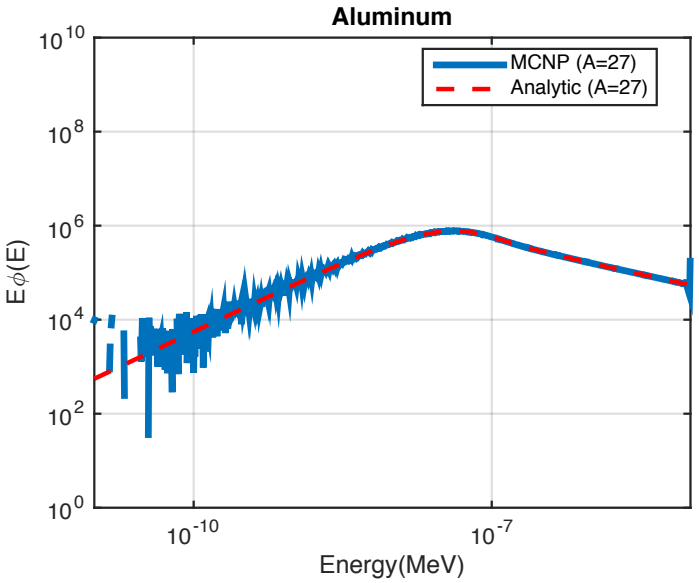
  - **Analytic benchmark for slowing down in an infinite medium, with elastic scattering – including free-gas scattering**
  - **First analytic benchmark (ever) to address free-gas scattering**
  - **Based on exact solution using heavy-gas model**
    - Does not apply for A=1
    - For large A, approaches 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 & Training

Monte Carlo Codes
XCP-3, LANL

- **User support**
  - **MCNP Forum - User-group, beginners & experts, ~ 1400 members**
  - **MCNP Website, MCNP Reference Collection**
  - **Summer students**
  - **Direct hands-on support for LANL NCS Division**
  - **Email consulting to many crit-safety analysts**
- **Classes**
  - **Theory & Practice of Criticality Calculations with MCNP**
    - 16 theory lectures (537 slides), 18 practical lectures (780 slides), 190 examples
    - FY14: 3 classes (2 LANL, 1 Hanford)
    - FY15: 3 classes (2 LANL, 1 Y-12)
    - FY16: 3 classes (2 LANL, 1 Sandia)
  - **Informal talks at LANL on validation & Whisper (~25 hrs, 262 slides)**
- **Conferences & Journals**
  - **M&C 2015, ICNC 2015, PHYSOR-2016**
  - **ANS …, Anaheim, San Antonio, Washington, …**
  - **OECD Expert Groups - Advanced Monte Carlo, Sensitivity/Uncertainty**

Work in Progress

Whisper – Validation & USLs

MCNP 2020 – Near-Term Targets

Other R&D Work, with Universities

Fission Neutron Multiplicity (Rising talk)

Whisper - Next Steps

- Portable version of Whisper & scripts [Brown]
- Revised User Manual for Whisper [Brown]
- Prepare Whisper training & demo [Brown, Alwin, Rising]
  - Slides & handouts
  - Demo
  - Follow-up ...
- Other Whisper mods & improvements [...]
- Prepare Whisper for distribution [Brown]
  - Other DOE crit-safety
  - MCNP release to RSICC
- Expand the Whisper benchmark suite [Alwin, NCS]
- Transition to MCNP6.2 [...]

MCNP 2020 – Progress

Monte Carlo Codes
XCP-3, LANL

MCNP 2020

- **Improve performance**
  - **Goal: 2X speedup within 2 years**
- **Upgrade core MCNP6 software**
  - **Evolution, not revolution**
  - **Restructure, clean up coding, standards compliance**
  - **Reorganize data structures**
  - **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**

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-15.0
  - gfortran-5.3

MCNP 2020 – Near-Term Targets

Monte Carlo Codes
XCP-3, LANL

NCSP-Related

- **Parallel threading** – measure 2015 performance of atomic-operations vs critical-sections; fully-threaded source
- **Examine memory allocation** – rearrange for better cache utilization
- **List tallies** – alternative tally scheme, to save memory & reduce lock/unlock overhead for threading
- **Light-weight cycle rendezvous for MPI calculations** – reduce unnecessary MPI messaging
- **Fission neutron multiplicity** – restructure & combine, ensure correct threading

Depending on non-NCSP funding

- **MPI improvements** – nonblocking messages, asynchronous transfers, in-place transfers, improved interface using Fortran-2003 polymorphism
- **Tally servers** – remote node storage for tallies with very large memory requirements
- **New standardized dump file** – direct access, access by dataset name, etc.
- **Upgrade for PTRAC & SSR** – permit use in parallel calculations, not just serial
- **HDF5 &/or MPI-IO** – improve read/write speed & portability of file output

Other R&D work, with Universities

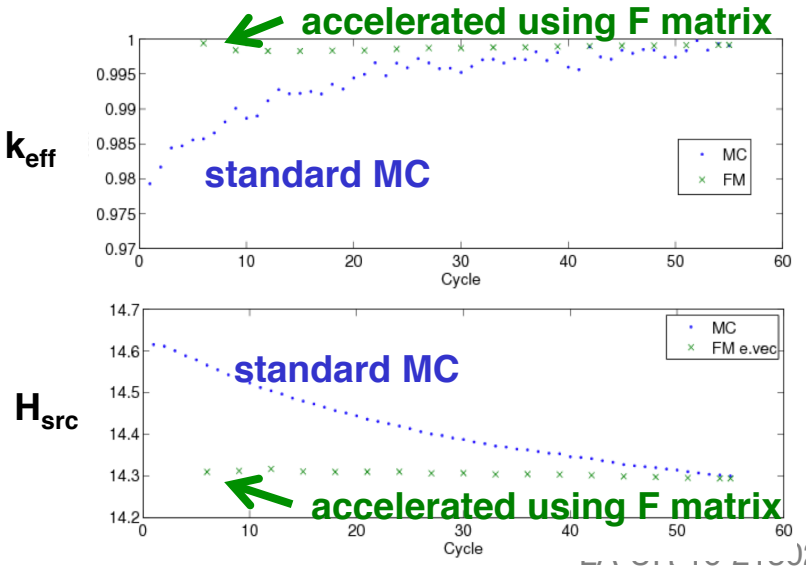
Monte Carlo Codes
XCP-3, LANL

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)
- Investigate coupling MCNP into multiphysics calculations (Michigan)
- V&V for using explicit fission neutron multiplicity distributions in criticality calculations (New Mexico)
- Doppler coefficients (New Mexico)

Fission Matrix

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



Summary

- MCNP6.1, MCNP6.1.1, & ENDF/B-VII.1 released
- Next release – TBD, probably Fall 2016

- 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

- Criticality-safety community needs to transition to MCNP6 over the next few years

Questions ?